Susan Hanley

Access DB# 79295

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: My-Chau Tram Examiner #: 78933 Date: 11/4/02
Art Unit: 1639 Phone Number 30 5-6999 Serial Number: 09/871,353
Mail Box and Bldg/Room Location: CM1, 8A16 Results Format Preferred (circle): PAPER DISK E-MAIL
6D38O1

If more than one search is submitted, please prioritize searches in order of need. 1ST

****

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: Functionalized Thiophene oligomers + their use as fluorescent markers

Inventors (please provide full names): Franco Cipriani; Giuseppe Gigli; Roberto Cingolani; Laura Favaretto; Massimo Zambianchi; Giovanna Sotgiu; Giovanna Barbarella; Gennaro Citro

Earliest Priority Filing Date: 5/31/00

**For Sequence Searches Only* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.*

Mrs. Hanley,

Please perform the following:

1) Inventor search
2) Search claim 1-13 (attached) especially keyword "thiophene oligomers"

Thanks!

Point of Contact
Susan Hanley
Technical Info. Specialist
CM1 6B05 Tel: 305-4053

STIC 11-4-02 CENTRAL

search history – a separate query display is attached to each answer set

TRAN 09/871,353

=> d his

```
     (FILE 'HOME' ENTERED AT 07:18:23 ON 20 NOV 2002)

     FILE 'HCAPLUS' ENTERED AT 07:18:34 ON 20 NOV 2002
L1            19 S CIPRIANI F?/AU
L2           135 S GIGLI G?/AU
L3           377 S CINGOLANI R?/AU
L4            48 S FAVARETTO L?/AU
L5            59 S ZAMBIANCHI M?/AU
L6            78 S SOTGIU G?/AU
L7            71 S CITRO G?/AU
L8           132 S BARBARELLA G?/AU
                 E DELL EMILIA/AU
                 E EMILIA/AU
                 E DELLEMILIA/AU
L9           734 S L1-8
L10           54 S L9 AND THIOPHENE
L11           30 S L10 AND OLIGOMER?
L12            5 S L11 AND (THIOPHENE OLIGOMER)/TI
                 SELECT RN L12 1-5

     FILE 'REGISTRY' ENTERED AT 07:23:58 ON 20 NOV 2002
L13           24 S E49-72

     FILE 'HCAPLUS' ENTERED AT 07:24:30 ON 20 NOV 2002
L14            4 S L12 AND L13
L15            5 S L12 OR L14

     FILE 'REGISTRY' ENTERED AT 07:25:45 ON 20 NOV 2002
                 SAVE L13 TRA353I/A TEMP

     FILE 'REGISTRY' ENTERED AT 07:56:41 ON 20 NOV 2002
L16                STR
L17        289013 S 16.145.3/RID
L18             0 S L16 SSS SAM SUB=L17
L19               STR L16
L20            18 S L19 SSS SAM SUB=L17
L21          5115 S L19 SSS FUL SUB=L17
                 SAVE L21 TEMP TRA353P/A
L22            50 S L16 SSS SAM SUB=L21
L23          2293 S L16 SSS FUL SUB=L21
                 SAVE L23 TRA353S1/A TEMP
L24               STR L16
L25          1242 S L24 SSS FUL SUB=L23
                 SAVE L25 TRA353S2/A TEMP
L26               STR L24
L27          1357 S L26 SSS FUL SUB=L23
                 SAVE L27 TEMP TRA353S3/A
L28           476 S L27 AND  3 16.145.3/RID
L29           166 S L27 AND  4 16.145.3/RID
L30           104 S L27 AND  5 16.145.3/RID
L31           746 S L28-30
L32           674 S L31 AND NC=1 NOT ("DIAZO" OR F/ELS)
L33         23948 S 2 16.145.3/RID
L34          6084 S L33 AND NR=2
L35          2996 S L33 AND "BITHIOPHENE"
L36          1089 S L35 AND ("HYDROXY" OR "HYDROXYL" OR "CARBOXALDEHYDE" OR "FORM
L37          1089 S L35 AND ("HYDROXY" OR "HYDROXYL" OR "CARBOXALDEHYDE" OR "FORM
```

Inventor search

5 citations selecting Reg # of cpds in L12 citations

24 cpds

5 citations w/ 24 cpds displayed

RID = Ring identifier for 

parent search 5,115 cpds having at least 3  joined together

subset #1 2293 cpds

subset # 2, 1357 cpds

3 thiophene rings

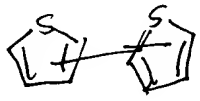
4 " " "

5 " " "

674 cpds w/ 3-5  rings and the claimed functional group of cl 4

bithiophene

Searched by Susan Hanley 305-4053

L33–40 is the search for 

TRAN 09/871,353

L38 searching for claim 4 functional grps & 2 [S] "amino" or "thiol" etc.

```
L38          662 S L35 AND ("HYDROXY" OR "HYDROXYL" OR "CARBOXALDEHYDE" OR "FORMY" OR
L39          584 S L38 AND NC=1
L40          451 S L39 NOT "AZO"

FILE 'HCAPLUS' ENTERED AT 08:40:12 ON 20 NOV 2002
L41          287 S L32
L42          455 S L40
L43           15 S L41(L)?CONJUGAT?
L44           14 S L42(L)?CONJUGAT?
L45           26 S L43 OR L44
L46           25 S L45 NOT L15
L47      3042811 S ANTIBOD? OR FLUORESC?(3A)MARKER OR PROTEIN OR DNA OR NUCLEIC
L48       121828 S SPECTROFLUORIMETRY OR CYTOMETRY OR FLUORESCENCE(W)MICROSCO? O
L49           40 S L41-42 AND L47-48
L50            8 S L49 AND ?CONJUGAT?
L51            7 S L50 NOT L15
L52           20 S L46 NOT L51
L53           18 S L52 NOT PATENT/DT
L54           17 S L53 AND PD<20010530
L55            4 S L54 AND (VISIBLE(3A)(UV OR ULTRAVIOET))
L56            2 S L52 AND PATENT/DT
L57           32 S L49 NOT (L50 OR L52)
L58            0 S L57 AND (VISIBLE(3A)(UV OR ULTRAVIOET))
L59           20 S L57 AND ?THIOPHEN?/OBI
L60           20 S L57 AND THIOPHEN?/OBI
L61           12 S L57 AND BITHIOPHEN?/OBI
L62            0 S L57 AND TRITHIOPHEN?/OBI
L63            0 S L57 AND TETRATHIOPHEN?/OBI
L64            0 S L57 AND PENTATHIOPHEN?/OBI
L65           21 S L60-61
L66            2 S L65 AND (?CONJUGAT? OR LINK? OR COVALENT? OR LIGAND)
L67           57 S L41-42 AND (VISIBLE(3A)(UV OR ULTRAVIOLET))
L68           52 S L67 NOT (L43 OR L45)
L69           15 S L68  AND (?CONJUGAT? OR LINK? OR COVALENT? OR LIGAND)
L70           15 S L69 NOT PATENT/DT
L71           14 S L70 AND PD<20010530

FILE 'REGISTRY' ENTERED AT 09:15:59 ON 20 NOV 2002
L72            6 S L32 AND  "ISOTHIOCYANATO"
L73            0 S L40 AND  "ISOTHIOCYANATO"
L74            0 S "BITHIOPHENE" AND  "ISOTHIOCYANATO"

FILE 'HCAPLUS' ENTERED AT 09:19:51 ON 20 NOV 2002
L75            2 S L72
L76            1 S L75 NOT L15
L77         1392 S OLIGOTHIOPHEN? OR OLIGOMER(3A)?THIOPHEN?
L78            2 S L77 AND ISOTHIOCYANAT?
L79            0 S L78 NOT L77
L80          745 S ?THIOPHEN? AND ISOTHIOCYANAT?
L81          264 S ?THIOPHEN?(L)ISOTHIOCYANAT?
L82            1 S L81(L)?CONJUGAT?
L83            2 S L81 AND ?CONJUGAT?
L84           19 S L81 AND (COVALENT? OR BIND? OR BOUND? OR LINK? OR LIGAND OR ?
L85            5 S L84 AND L47-48

FILE 'STNGUIDE' ENTERED AT 09:26:29 ON 20 NOV 2002
```

NC = # components

451 cpds w/ 2 [S] & 4 functional groups

287 cites for 3-5 thiophene rings

455 cites for bithiophene rings

Claimed uses

7 cites for L40 or L32 oligomers & conjugat. & claimed uses

4 cites

2 cites

2 cites

14 citations

L72-76 looking for oligothiophene w/ S=C=N group

1 cite (applicant) ☆ this specie is disclosed only by applicant ☆

appl. stuff

not useful

L77-85 - term searching - didn't yield anything new or useful

Searched by Susan Hanley 305-4053

STR for cpds w/ 3-5  & a functional group

TRAN 09/871,353

=> d que 141
L16 STR

subset #1

Hy = 

G1 = these functional groups.
Q = hetero atom
A = non-hydrogen atom

G1 must be present (connected) to the Hy – Hy – Hy STR

VAR G1=5/6/8/12/NH2/OH/SH/SO3H/SO2
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
GGCAT IS MCY UNS AT 1
GGCAT IS MCY UNS AT 2
GGCAT IS MCY UNS AT 3
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS E4 C E1 S AT 1
ECOUNT IS E4 C E1 S AT 2
ECOUNT IS E4 C E1 S AT 3

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE
L17 289013 SEA FILE=REGISTRY ABB=ON PLU=ON 16.145.3/RID ← parent set ← L1 was searched against
L19 STR

parent STR

Hy Hy Hy
1 2 3

Hy = 

must be at least 3 thiophenes

NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
GGCAT IS MCY UNS AT 1
GGCAT IS MCY UNS AT 2
GGCAT IS MCY UNS AT 3
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS E4 C E1 S AT 1
ECOUNT IS E4 C E1 S AT 2
ECOUNT IS E4 C E1 S AT 3

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 3

STEREO ATTRIBUTES: NONE
L21 5115 SEA FILE=REGISTRY SUB=L17 SSS FUL L19 — 5115 cpds for parent STR
L23 2293 SEA FILE=REGISTRY SUB=L21 SSS FUL L16 — 2293 cpds from subset STR #1
L26 STR

Subset STR #2

(over)

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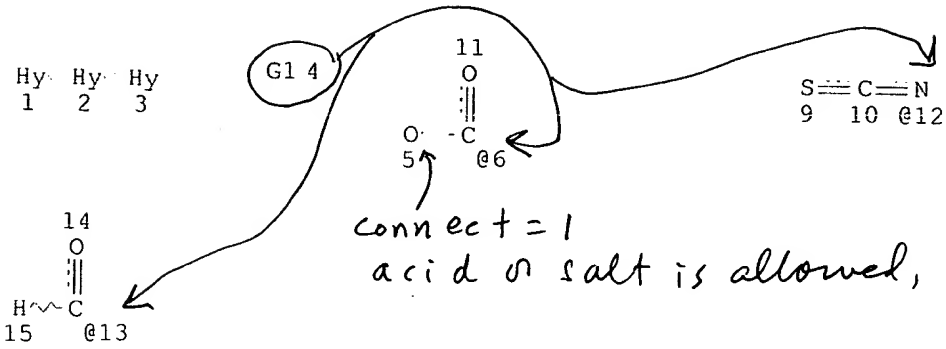
Subset STR #2 TRAN 09/871,353



connect = 1
acid or salt is allowed, no esters

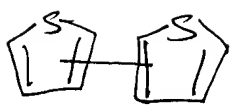
VAR G1=OH/SH/NH2/13/6/12 ← claim 4 functional groups
NODE ATTRIBUTES:
CONNECT IS E1 RC AT 5
DEFAULT MLEVEL IS ATOM
GGCAT IS MCY UNS AT 1
GGCAT IS MCY UNS AT 2
GGCAT IS MCY UNS AT 3
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS E4 C E1 S AT 1
ECOUNT IS E4 C E1 S AT 2
ECOUNT IS E4 C E1 S AT 3

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE
L27 1357 SEA FILE=REGISTRY SUB=L23 SSS FUL L26 1357 cpds from subset #2
L28 476 SEA FILE=REGISTRY ABB=ON PLU=ON L27 AND 3 16.145.3/RID 3 thio phens
L29 166 SEA FILE=REGISTRY ABB=ON PLU=ON L27 AND 4 16.145.3/RID 4 " "
L30 104 SEA FILE=REGISTRY ABB=ON PLU=ON L27 AND 5 16.145.3/RID 5 " "
L31 746 SEA FILE=REGISTRY ABB=ON PLU=ON (L28 OR L29 OR L30)
L32 674 SEA FILE=REGISTRY ABB=ON PLU=ON L31 AND NC=1 NOT ("DIAZO" OR F/ELS) 674 cpds
L41 287 SEA FILE=HCAPLUS ABB=ON PLU=ON L32 287 cites for L32 cpds

Searched by Susan Hanley 305-4053

search for: bithiophenes



TRAN 09/871,353

Ring ID for ↑

```
=> d que l42
L33         23948 SEA FILE=REGISTRY ABB=ON  PLU=ON  2|16.145.3/RID|
L35          2996 SEA FILE=REGISTRY ABB=ON  PLU=ON  L33 AND "BITHIOPHENE"
L38           662 SEA FILE=REGISTRY ABB=ON  PLU=ON  L35 AND ("HYDROXY" OR
                  "HYDROXYL" OR "CARBOXALDEHYDE" OR "FORMYL" OR  "ISOTHIOCYANATO"
                   OR "THIOL" OR "AMINO" OR "CARBOXYLIC") NOT "ESTER"
L39           584 SEA FILE=REGISTRY ABB=ON  PLU=ON  L38 AND NC=1
L40           451 SEA FILE=REGISTRY ABB=ON  PLU=ON  L39 NOT "AZO"
L42           455 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L40
```

functional groups

451 cpds w/

455 cites for L40 cpds

2  = a functional group

Searched by Susan Hanley 305-4053

Inventor search

TRAN 09/871,353

```
=> d que l15
L1          19 SEA FILE=HCAPLUS ABB=ON  PLU=ON  CIPRIANI F?/AU
L2         135 SEA FILE=HCAPLUS ABB=ON  PLU=ON  GIGLI G?/AU
L3         377 SEA FILE=HCAPLUS ABB=ON  PLU=ON  CINGOLANI R?/AU
L4          48 SEA FILE=HCAPLUS ABB=ON  PLU=ON  FAVARETTO L?/AU
L5          59 SEA FILE=HCAPLUS ABB=ON  PLU=ON  ZAMBIANCHI M?/AU
L6          78 SEA FILE=HCAPLUS ABB=ON  PLU=ON  SOTGIU G?/AU
L7          71 SEA FILE=HCAPLUS ABB=ON  PLU=ON  CITRO G?/AU
L8         132 SEA FILE=HCAPLUS ABB=ON  PLU=ON  BARBARELLA G?/AU
L9         734 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L1 OR L2 OR L3 OR L4 OR L5
                OR L6 OR L7 OR L8)
L10         54 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L9 AND THIOPHENE
L11         30 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L10 AND OLIGOMER?
L12          5 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L11 AND (THIOPHENE OLIGOMER)/T
                I
L13         24 SEA FILE=REGISTRY ABB=ON  PLU=ON  (376393-41-8/BI OR 376393-42-
                9/BI OR 376393-43-0/BI OR 376393-44-1/BI OR 492-97-7/BI OR
                111372-97-5/BI OR 111744-23-1/BI OR 113386-74-6/BI OR 116159-99
                -0/BI OR 118347-89-0/BI OR 127236-47-9/BI OR 127236-48-0/BI OR
                127473-73-8/BI OR 127473-74-9/BI OR 127473-75-0/BI OR 139747-07
                -2/BI OR 139747-08-3/BI OR 14762-74-4/BI OR 201604-95-7/BI OR
                201604-98-0/BI OR 25233-34-5/BI OR 376393-45-2/BI OR 5632-29-1/
                BI OR 67984-20-7/BI)
L14          4 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L12 AND L13
L15          5 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L12 OR L14
```

5 citations

searching Reg # from L12 cites -24 cpds

5 cites w/ 24 cpds displayed

Searched by Susan Hanley 305-4053

=> d ibib abs hitstr ind 1

L15 ANSWER 1 OF 5 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2002:851250 HCAPLUS
TITLE: Solvent-Free, Microwave-Assisted Synthesis of **Thiophene Oligomers** via Suzuki Coupling
AUTHOR(S): Melucci, Manuela; **Barbarella, Giovanna; Sotgiu, Giovanna**
CORPORATE SOURCE: Consiglio Nazionale Ricerche (ISOF), Bologna, 40129, Italy
SOURCE: Journal of Organic Chemistry ACS ASAP
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The purpose of this study was to obtain a rapid, efficient, and environmentally friendly methodol. for the synthesis of highly pure **thiophene oligomers**. The solvent-free, microwave-assisted coupling of thienyl boronic acids and esters with thienyl bromides, using aluminum oxide as the solid support, allowed us to rapidly check the reaction trends on changing times, temp., catalyst, and base and easily optimize the exptl. conditions to obtain the targeted product in fair amts. This procedure offers a novel, general, and very rapid route to the prepn. of sol. **thiophene oligomers**. Thus, for example, quaterthiophene was obtained in 6 min by reaction of 2-bromo-2,2'-bithiophene with bis(pinacolato)diboron (isolated yield 65%), whereas quinquethiophene was obtained in 11 min by reaction of dibromoterthiophene with thienylboronic acid (isolated yield 74%). The synthesis of new chiral 2,2'-bithiophenes is reported. The detailed anal. of the byproducts of some reactions allowed us to elucidate a few aspects of reaction mechanisms. While the use of microwaves proved to be very convenient for the coupling between conventional thienyl moieties, the same was not true for the coupling of thienyl rings to thienyl-S,S-dioxide moieties. Indeed, in this case, the targeted product was obtained in low yields because of the competitive, accelerated, Diels-Alder reaction that affords a variety of condensation products.

CC 35 (Chemistry of Synthetic High Polymers)

=> d ibib abs hitstr ind 2

L15 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:885415 HCAPLUS
DOCUMENT NUMBER: 136:2509
TITLE: Functionalized **thiophene oligomers** and their use as fluorescent markers
INVENTOR(S): **Cipriani, Franco; Gigli, Giuseppe; Cingolani, Roberto; Favaretto, Laura ; Zambianchi, Massimo; Sotgiu, Giovanna; Barbarella, Giovanna; Citro, Gennaro**
PATENT ASSIGNEE(S): Consiglio Nazionale Delle Ricerche, Italy; Istituto Nazionale Per La Fisica Della Materia; Bio-D S.R.L.
SOURCE: Eur. Pat. Appl., 9 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

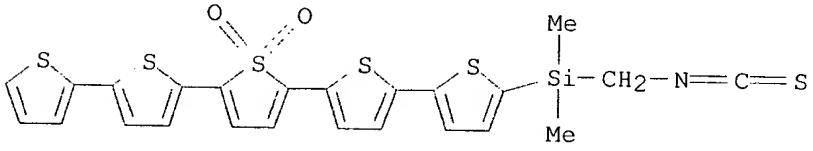
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1160246	A2	20011205	EP 2001-113236	20010530
EP 1160246	A3	20020130		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
US 2002086437	A1	20020704	US 2001-871353	20010530

PRIORITY APPLN. INFO.: IT 2000-BA20 A 20000531

AB The invention concerns the synthesis of **thiophene oligomers** and their use as fluorescent markers in anal. techniques. The **oligomers** are excitable in the visible and UV region and have at least one functional group able to form a covalent bond with org. and/or biol. mols., so as not to alter either the fluorescence properties of the **oligomers** or the biol. activity of the bound mols.

IT **376393-44-1D**, conjugates with proteins
RL: ANT (Analyte); ANST (Analytical study)
(functionalized **thiophene oligomers** and use as fluorescent markers)

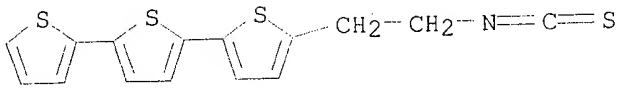
RN 376393-44-1 HCAPLUS
CN Silane, (1'',1''-dioxido[2,2':5',2'':5'',2''':5''',2''''-quinquethiophen]-5-yl)(isothiocyanatomethyl)dimethyl- (9CI) (CA INDEX NAME)



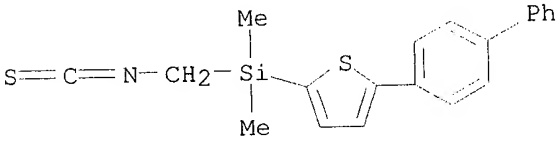
IT **376393-41-8P 376393-42-9P 376393-43-0P 376393-44-1P**
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
(functionalized **thiophene oligomers** and use as fluorescent markers)

RN 376393-41-8 HCAPLUS

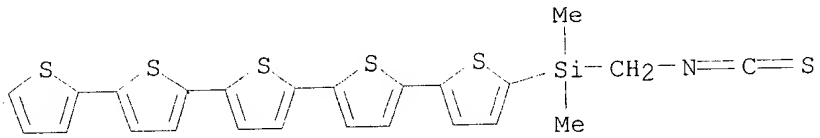
CN 2,2':5',2''-Terthiophene, 5-(2-isothiocyanatoethyl)- (9CI) (CA INDEX NAME)



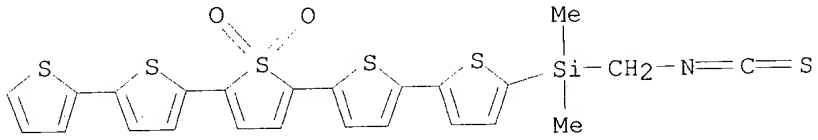
RN 376393-42-9 HCAPLUS
CN Silane, (5-[1,1'-biphenyl]-4-yl-2-thienyl)(isothiocyanatomethyl)dimethyl- (9CI) (CA INDEX NAME)



RN 376393-43-0 HCAPLUS
CN Silane, (isothiocyanatomethyl)dimethyl[2,2':5',2'':5'',2''':5''',2''''-quinquethiophen]-5-yl- (9CI) (CA INDEX NAME)

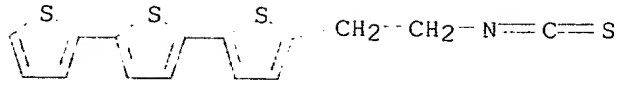


RN 376393-44-1 HCAPLUS
CN Silane, (1'',1'''-dioxido[2,2':5',2'':5'',2''':5''',2''''-quinquethiophen]-5-yl)(isothiocyanatomethyl)dimethyl- (9CI) (CA INDEX NAME)

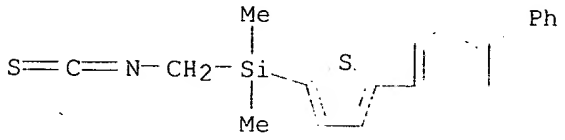


IT **376393-41-8DP**, conjugates with proteins **376393-42-9DP**, conjugates with proteins **376393-43-0DP**, conjugates with monoclonal anti-CD8 antibody **376393-45-2DP**, conjugates with albumin
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(functionalized **thiophene oligomers** and use as fluorescent markers)

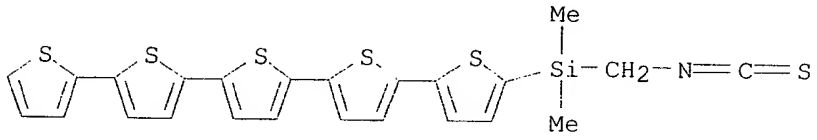
RN 376393-41-8 HCAPLUS
CN 2,2':5',2''-Terthiophene, 5-(2-isothiocyanatoethyl)- (9CI) (CA INDEX NAME)



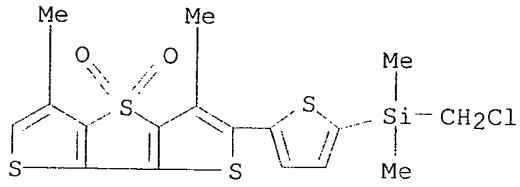
RN 376393-42-9 HCAPLUS
CN Silane, (5-[1,1'-biphenyl]-4-yl-2-thienyl)(isothiocyanatomethyl)dimethyl- (9CI) (CA INDEX NAME)



RN 376393-43-0 HCAPLUS
CN Silane, (isothiocyanatomethyl)dimethyl[2,2':5',2'':5'',2''':5''',2''''-quinquethiophen]-5-yl- (9CI) (CA INDEX NAME)



RN 376393-45-2 HCAPLUS
CN Silane, (chloromethyl)[5-(3,5-dimethyl-4,4-dioxidodithieno[3,2-b:2',3'-d]thien-2-yl)-2-thienyl]dimethyl- (9CI) (CA INDEX NAME)



IC ICM C07D333-20
ICS C07D333-48; C07F007-08; G01N033-53
CC 9-14 (Biochemical Methods)
ST **thiophene oligomer** fluorescence marker protein isothiocyanate fluorometry biol analysis
IT Proteins
RL: ANT (Analyte); PRP (Properties); ANST (Analytical study)
(conjugates with synthesized **thiophene oligomers**; functionalized **thiophene oligomers** and use as fluorescent markers)
IT Cytometry
(flow; functionalized **thiophene oligomers** and use as fluorescent markers)
IT Immunoglobulins
RL: ANT (Analyte); ANST (Analytical study)
(fragments; functionalized **thiophene oligomers** and

use as fluorescent markers)

IT Amide group
Carbonyl group
Carboxyl group
Fluorescence microscopy
Fluorescent substances
Fluorometry
Formyl group
Functional groups
Gel electrophoresis
Pharmaceutical analysis
Sulfhydryl group
T cell (lymphocyte)
UV and visible spectroscopy
(functionalized **thiophene oligomers** and use as fluorescent markers)

IT Hormones, animal, analysis
Neurotransmitters
Nucleic acids
Oligonucleotides
Proteins
RL: ANT (Analyte); ANST (Analytical study)
(functionalized **thiophene oligomers** and use as fluorescent markers)

IT Functional groups
(isothiocyanato group; functionalized **thiophene oligomers** and use as fluorescent markers)

IT Antibodies
RL: ANT (Analyte); ANST (Analytical study)
(monoclonal, CD8; functionalized **thiophene oligomers** and use as fluorescent markers)

IT **376393-44-1D**, conjugates with proteins
RL: ANT (Analyte); ANST (Analytical study)
(functionalized **thiophene oligomers** and use as fluorescent markers)

IT **376393-41-8P 376393-42-9P 376393-43-0P 376393-44-1P**
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
(functionalized **thiophene oligomers** and use as fluorescent markers)

IT **376393-41-8DP**, conjugates with proteins **376393-42-9DP**, conjugates with proteins **376393-43-0DP**, conjugates with monoclonal anti-CD8 antibody **376393-45-2DP**, conjugates with albumin
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(functionalized **thiophene oligomers** and use as fluorescent markers)

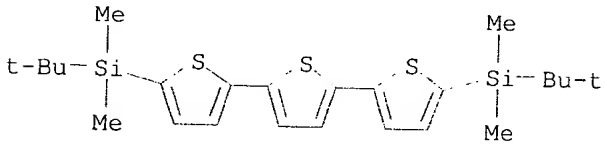
=> d ibib abs hitstr ind 3

L15 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1998:686632 HCAPLUS
DOCUMENT NUMBER: 130:25513
TITLE: Structural and Electrical Characterization of Processable Bis-Silylated **Thiophene Oligomers**
AUTHOR(S): **Barbarella, G.**; Ostoja, P.; Maccagnani, P.; Pudova, Olga; Antolini, L.; Casarini, D.; Bongini, A.
CORPORATE SOURCE: I.Co.C.E.A. L.A.M.E.L., Consiglio Nazionale Ricerche, Bologna, 40129, Italy
SOURCE: Chemistry of Materials (1998), 10(11), 3683-3689
CODEN: CMATEX; ISSN: 0897-4756
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

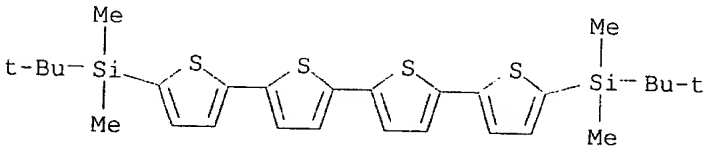
AB A new class of processable, chem. stable, and easily synthesized and purified .alpha.,.omega.-bis(dimethyl-tert-butylsilyl) oligothiophenes is described. Information on the solid-state properties was obtained by single crystal X-ray diffraction and CPMAS NMR spectroscopy. Mol. packing was characterized by a sandwich-type organization, with the mol. planes between adjacent layers along the stacking direction being exactly parallel. Vacuum-evapd. thin films of the tetramer, pentamer, and hexamer displayed field effect transistor activity, with charge mobilities increasing with the substrate deposition temps. in the range 28-80 .degree.C. The best FET performance was achieved with the pentamer which was characterized by an on/off ratio > 103, reproducibility, and a device stability in air of months.

IT **201604-95-7 201604-98-0**
RL: PRP (Properties)
(structural and elec. characterization of processable bis-silylated **thiophene oligomers**)

RN 201604-95-7 HCAPLUS
CN Silane, 2,2':5',2''-terthiophene-5,5''-diylbis[(1,1-dimethylethyl)dimethyl- (9CI) (CA INDEX NAME)



RN 201604-98-0 HCAPLUS
CN Silane, 2,2':5',2'':5'',2'''-quaterthiophene-5,5'''-diylbis[(1,1-dimethylethyl)dimethyl- (9CI) (CA INDEX NAME)



CC 36-2 (Physical Properties of Synthetic High Polymers)
Section cross-reference(s): 76

ST bis silylated **thiophene oligomer** structure elec property

IT MAS NMR spectroscopy
(CP; structural and elec. characterization of processable bis-silylated **thiophene oligomers**)

IT Polymers, properties
RL: PRP (Properties)
(polythiophenes, **oligomeric**, silane-terminated; structural and elec. characterization of processable bis-silylated **thiophene oligomers**)

IT Crystal structure
Field effect transistors
Polymer chains
(structural and elec. characterization of processable bis-silylated **thiophene oligomers**)

IT **201604-95-7 201604-98-0**
RL: PRP (Properties)
(structural and elec. characterization of processable bis-silylated **thiophene oligomers**)

REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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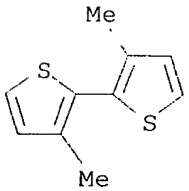
L15 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1992:150890 HCAPLUS
DOCUMENT NUMBER: 116:150890
TITLE: Conformation and optical absorption properties of **thiophene oligomers**: carbon-13 NMR, UV, and MMP2 calculations of di- and tetramethylquaterthiophenes
AUTHOR(S): **Barbarella, Giovanna**; Bongini, Alessandro; **Zambianchi, Massimo**
CORPORATE SOURCE: Inst. Composti Carbonio Contenenti Eteroatomi Loro Appl., Ozzano Emilia, I-40066, Italy
SOURCE: Advanced Materials (Weinheim, Germany) (1991), 3(10), 494-6
CODEN: ADVMEW; ISSN: 0935-9648
DOCUMENT TYPE: Journal
LANGUAGE: English

AB 13C NMR and UV data, together with MMP2 calcns., indicate that the degree of planarity of quaterthiophenes in soln. is given by the cis junctions between adjacent rings ant that only the presence of 2 Me in the 3,3' positions of a bithiophene subsystem freezes the conformation in the anti orientation, leading to the system being markedly non-planar.

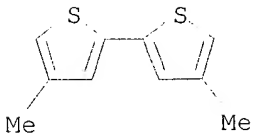
IT **492-97-7**, 2,2'-Bithiophene **67984-20-7**
111372-97-5 113386-74-6 116159-99-0
118347-89-0 127236-48-0 139747-08-3
RL: PRP (Properties)
(carbon-13 NMR and UV of, conjugation and)

RN 492-97-7 HCAPLUS
CN 2,2'-Bithiophene (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

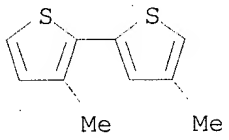
RN 67984-20-7 HCAPLUS
CN 2,2'-Bithiophene, 3,3'-dimethyl- (6CI, 9CI) (CA INDEX NAME)



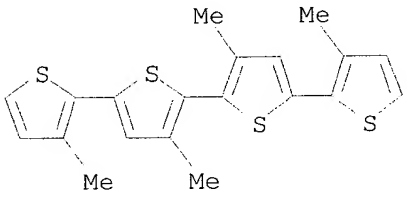
RN 111372-97-5 HCAPLUS
CN 2,2'-Bithiophene, 4,4'-dimethyl- (9CI) (CA INDEX NAME)



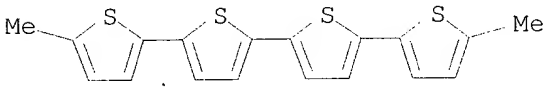
RN 113386-74-6 HCAPLUS
CN 2,2'-Bithiophene, 3,4'-dimethyl- (9CI) (CA INDEX NAME)



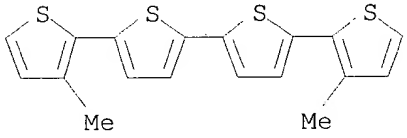
RN 116159-99-0 HCAPLUS
CN 2,2':5',2'':5'',2'''-Quaterthiophene, 3,3'',3''',4'-tetramethyl- (9CI) (CA INDEX NAME)



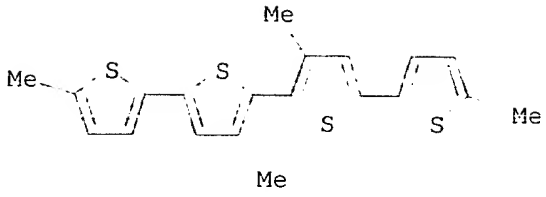
RN 118347-89-0 HCAPLUS
CN 2,2':5',2'':5'',2'''-Quaterthiophene, 5,5'''-dimethyl- (9CI) (CA INDEX NAME)



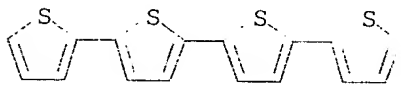
RN 127236-48-0 HCAPLUS
CN 2,2':5',2'':5'',2'''-Quaterthiophene, 3,3'''-dimethyl- (9CI) (CA INDEX NAME)



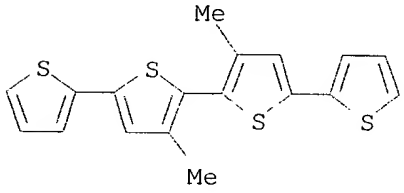
RN 139747-08-3 HCAPLUS
CN 2,2':5',2'':5'',2'''-Quaterthiophene, 3'',4',5,5'''-tetramethyl- (9CI) (CA INDEX NAME)



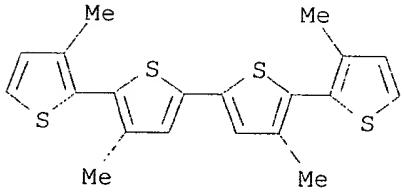
IT **5632-29-1**, Quaterthiophene **127236-47-9**
139747-07-2
RL: PRP (Properties)
(carbon-13 NMR in UV, mol. mechanics, and conformation of, conjugation and)
RN 5632-29-1 HCAPLUS
CN 2,2':5',2'':5'',2'''-Quaterthiophene (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 127236-47-9 HCAPLUS
CN 2,2':5',2'':5'',2'''-Quaterthiophene, 3'',4'-dimethyl- (9CI) (CA INDEX NAME)



RN 139747-07-2 HCAPLUS
CN 2,2':5',2'':5'',2'''-Quaterthiophene, 3,3',3''',4''-tetramethyl- (9CI) (CA INDEX NAME)



IT **14762-74-4**
RL: PRP (Properties)
(nuclear magnetic resonance, of quaterthiophene and related compds., carbon-13)
RN 14762-74-4 HCAPLUS
CN Carbon, isotope of mass 13 (8CI, 9CI) (CA INDEX NAME)

^{13}C

CC 22-3 (Physical Organic Chemistry)
ST UV methylquaterthiophene; carbon NMR methylquaterthiophene; conformation methylquaterthiophene mol mechanism
IT Methyl group
(effect of, on conformation of quaterthiophene and related compds.)
IT Conjugation
Hyperconjugation
(in quaterthiophene and related compds.)
IT Conformation and Conformers
(of quaterthiophene and related compds.)
IT Nuclear magnetic resonance
(of quaterthiophene and related compds., carbon-13)
IT Molecular mechanics
(of quaterthiophene and related compds., conformation and)
IT Ultraviolet and visible spectra
(of quaterthiophene and related compds., conjugation and)
IT **492-97-7**, 2,2'-Bithiophene **67984-20-7** **111372-97-5** **113386-74-6** **116159-99-0** **118347-89-0** **127236-48-0** **139747-08-3**
RL: PRP (Properties)
(carbon-13 NMR and UV of, conjugation and)
IT **5632-29-1**, Quaterthiophene **127236-47-9** **139747-07-2**
RL: PRP (Properties)
(carbon-13 NMR in UV, mol. mechanics, and conformation of, conjugation and)
IT **14762-74-4**
RL: PRP (Properties)
(nuclear magnetic resonance, of quaterthiophene and related compds., carbon-13)

=> d ibib abs hitstr ind 5

L15 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1990:460286 HCAPLUS
DOCUMENT NUMBER: 113:60286
TITLE: Determination of the electronic structure of **thiophene oligomers** and extrapolation to polythiophene
AUTHOR(S): Jones, Derek; Guerra, Maurizio; **Favaretto, Laura**; Modelli, Alberto; Fabrizio, Monica; Distefano, Giuseppe
CORPORATE SOURCE: ICoCEA, Cons. Naz. Ric., Ozzano Emilia, 40064, Italy
SOURCE: Journal of Physical Chemistry (1990), 94(15), 5761-6
CODEN: JPCHAX; ISSN: 0022-3654
DOCUMENT TYPE: Journal
LANGUAGE: English

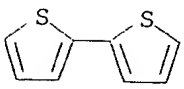
AB Ionization energies, attachment energies, and electrochem. redn. potentials of **thiophene oligomers** (d.p. .ltoreq.5) were detd. exptl. (UV photoelectron and electron transmission spectroscopies and cyclic voltammetry) and theor. (ionization and attachment energies by MINDO/3). The geometrical parameters of the most stable conformation of 2,2'-bithienyl were computed at the ab initio STO-3G level with complete relaxation. A short extrapolation of the energy data to the polymer provided accurate and reliable values for important properties of polythiophene in the gas phase, namely: ionization energy 6.9 eV, valence bandwidth 3.2 eV, electron affinity 0.9.apprx.1.1 eV, HOMO-LUMO energy gap 5.9 eV, and .lambda.max 2.7 eV.

IT **25233-34-5, Thiophene** homopolymer
RL: PRP (Properties)
(electronic structure of, electronic structure of **oligomers** in relation to)
RN 25233-34-5 HCAPLUS
CN Thiophene, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 110-02-1
CMF C4 H4 S

IT **492-97-7**, 2,2'-Bithiophene **111744-23-1**, Terthiophene **127473-73-8 127473-74-9 127473-75-0**
RL: PRP (Properties)
(electronic structure of, polythiophene electronic structure in relation to)
RN 492-97-7 HCAPLUS
CN 2,2'-Bithiophene (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 111744-23-1 HCAPLUS
CN Terthiophene (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 127473-73-8 HCAPLUS
CN Thiophene, tetramer (9CI) (CA INDEX NAME)

CM 1

CRN 110-02-1
CMF C4 H4 S

RN 127473-74-9 HCAPLUS
CN Thiophene, pentamer (9CI) (CA INDEX NAME)

CM 1

CRN 110-02-1
CMF C4 H4 S

RN 127473-75-0 HCAPLUS
CN Thiophene, hexamer (9CI) (CA INDEX NAME)

CM 1

CRN 110-02-1
CMF C4 H4 S

CC 36-5 (Physical Properties of Synthetic High Polymers)
ST **thiophene oligomer** polymer electronic structure; ionization energy **thiophene oligomer** polymer; attachment energy **thiophene oligomer** polymer; electrochem redn potential **thiophene oligomer**; conformation **thiophene oligomer** polymer; valence bandwidth **thiophene oligomer**; electron affinity **thiophene oligomer** polymer; energy gap **thiophene oligomer** polymer
IT Chains, chemical
(conformation of, in **thiophene oligomers**)
IT Ionization potential and energy
(of **thiophene oligomers**, electronic structure of polythiophene in relation to)

IT Electron affinity
(of **thiophene oligomers**, electronic structure of **thiophene** polymers in relation to)
IT Molecular orbital
(MINDO/3, of **thiophene oligomers**)
IT Molecular orbital
(frontier, of **thiophene oligomers**)
IT Energy level, band structure
(gap, of **thiophene oligomers**, polythiophene electronic structure in relation to)
IT Electric potential
(redn., of **thiophene oligomers**, electronic structure of polythiophene in relation to)
IT Energy level, band structure
(valence, of **thiophene oligomers**, electronic structure of polythiophene in relation to)
IT **25233-34-5**, **Thiophene** homopolymer
RL: PRP (Properties)
(electronic structure of, electronic structure of **oligomers** in relation to)
IT **492-97-7**, 2,2'-Bithiophene **111744-23-1**, Terthiophene **127473-73-8** **127473-74-9** **127473-75-0**
RL: PRP (Properties)
(electronic structure of, polythiophene electronic structure in relation to)

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L2         135 SEA FILE=HCAPLUS ABB=ON  PLU=ON  GIGLI G?/AU
L3         377 SEA FILE=HCAPLUS ABB=ON  PLU=ON  CINGOLANI R?/AU
L4          48 SEA FILE=HCAPLUS ABB=ON  PLU=ON  FAVARETTO L?/AU
L5          59 SEA FILE=HCAPLUS ABB=ON  PLU=ON  ZAMBIANCHI M?/AU
L6          78 SEA FILE=HCAPLUS ABB=ON  PLU=ON  SOTGIU G?/AU
L7          71 SEA FILE=HCAPLUS ABB=ON  PLU=ON  CITRO G?/AU
L8         132 SEA FILE=HCAPLUS ABB=ON  PLU=ON  BARBARELLA G?/AU
L9         734 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L1 OR L2 OR L3 OR L4 OR L5
               OR L6 OR L7 OR L8)
L10         54 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L9 AND THIOPHENE
L11         30 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L10 AND OLIGOMER?
L12          5 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L11 AND (THIOPHENE OLIGOMER)/T
               I
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               -0/BI OR 118347-89-0/BI OR 127236-47-9/BI OR 127236-48-0/BI OR
               127473-73-8/BI OR 127473-74-9/BI OR 127473-75-0/BI OR 139747-07
               -2/BI OR 139747-08-3/BI OR 14762-74-4/BI OR 201604-95-7/BI OR
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               BI OR 67984-20-7/BI)
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L15          5 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L12 OR L14
L16            STR
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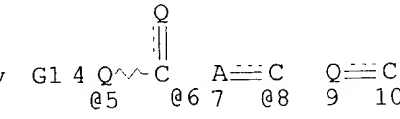
inv. search

5 cites from applicants

1st Subset STR

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GGCAT   IS MCY  UNS  AT   3
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ECOUNT  IS E4 C  E1 S  AT   2
ECOUNT  IS E4 C  E1 S  AT   3

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  12

STEREO ATTRIBUTES: NONE
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L19            STR
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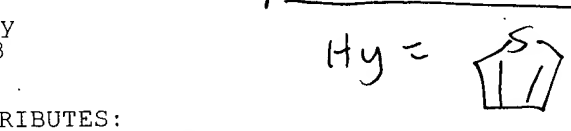
parent search

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Searched by Susan Hanley 305-4053

the STR search to obtain L32 answer set (cpds w/ 3-5 [S] [1]) & term search to get L45 (bi thiophene

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ECOUNT  IS E4 C  E1 S  AT   3

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   3

STEREO ATTRIBUTES: NONE
L21         5115 SEA FILE=REGISTRY SUB=L17 SSS FUL L19
L23         2293 SEA FILE=REGISTRY SUB=L21 SSS FUL L16
L26              STR
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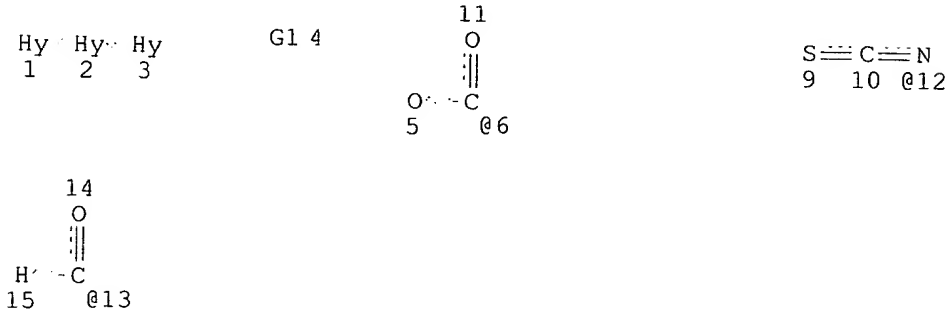
2nd subset STR

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VAR G1=OH/SH/NH2/13/6/12
NODE ATTRIBUTES:
CONNECT IS E1  RC AT   5
DEFAULT MLEVEL IS ATOM
GGCAT   IS MCY  UNS  AT   1
GGCAT   IS MCY  UNS  AT   2
GGCAT   IS MCY  UNS  AT   3
DEFAULT ECLEVEL IS LIMITED
ECOUNT  IS E4 C  E1 S  AT   1
ECOUNT  IS E4 C  E1 S  AT   2
ECOUNT  IS E4 C  E1 S  AT   3

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  13

STEREO ATTRIBUTES: NONE
L27         1357 SEA FILE=REGISTRY SUB=L23 SSS FUL L26
L28          476 SEA FILE=REGISTRY ABB=ON  PLU=ON  L27 AND  3 16.145.3/RID
L29          166 SEA FILE=REGISTRY ABB=ON  PLU=ON  L27 AND  4 16.145.3/RID
L30          104 SEA FILE=REGISTRY ABB=ON  PLU=ON  L27 AND  5 16.145.3/RID
L31          746 SEA FILE=REGISTRY ABB=ON  PLU=ON  (L28 OR L29 OR L30)
L32          674 SEA FILE=REGISTRY ABB=ON  PLU=ON  L31 AND NC=1 NOT ("DIAZO" OR
                 F/ELS)
L33        23948 SEA FILE=REGISTRY ABB=ON  PLU=ON  2 16.145.3/RID
L35         2996 SEA FILE=REGISTRY ABB=ON  PLU=ON  L33 AND "BITHIOPHENE"
L38          662 SEA FILE=REGISTRY ABB=ON  PLU=ON  L35 AND ("HYDROXY" OR
                 "HYDROXYL" OR "CARBOXALDEHYDE" OR "FORMYL" OR  "ISOTHIOCYANATO"
                  OR "THIOL" OR "AMINO" OR "CARBOXYLIC") NOT "ESTER"
L39          584 SEA FILE=REGISTRY ABB=ON  PLU=ON  L38 AND NC=1
L40          451 SEA FILE=REGISTRY ABB=ON  PLU=ON  L39 NOT "AZO"
L41          287 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L32
```

674 cpds

3-5 S [5] rings

451 cpds w/ 2 [5]

287 cites for L32 cpds

Searched by Susan Hanley 305-4053

TRAN 09/871,353

L42	455	SEA FILE=HCAPLUS ABB=ON PLU=ON L40
L47	3042811	SEA FILE=HCAPLUS ABB=ON PLU=ON ANTIBOD? OR FLUORESC?(3A)MARKER OR PROTEIN OR DNA OR NUCLEIC OR OLIGONUC? OR HORMON? OR DRUG OR MEDICINE OR NEUROTRANSMITTER
L48	121828	SEA FILE=HCAPLUS ABB=ON PLU=ON SPECTROFLUORIMETRY OR CYTOMETRY OR FLUORESCENCE(W)MICROSCO? OR GEL ELECTROPHOR?
L49	40	SEA FILE=HCAPLUS ABB=ON PLU=ON (L41 OR L42) AND (L47 OR L48)
L50	8	SEA FILE=HCAPLUS ABB=ON PLU=ON L49 AND ?CONJUGAT?
L51	7	SEA FILE=HCAPLUS ABB=ON PLU=ON L50 NOT L15

455 cites for 2 [5] [1]

7 cites

subtracting out applicant's work

Searched by Susan Hanley 305-4053

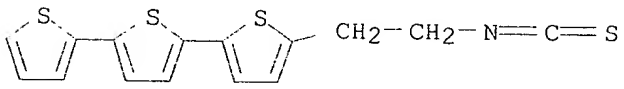
=> d ibib abs hitstr 1

L51 ANSWER 1 OF 7 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:792698 HCAPLUS
DOCUMENT NUMBER: 136:66480
TITLE: Oligothiophene isothiocyanates as a new class of **fluorescent markers** for biopolymers
AUTHOR(S): Barbarella, Giovanna; Zambianchi, Massimo; Pudova, Olga; Paladini, Vanessa; Ventola, Alfredo; Cipriani, Francesco; Gigli, Giuseppe; Cingolani, Roberto; Citro, Gennaro
CORPORATE SOURCE: Consiglio Nazionale Ricerche, I.Co.C.E.A, Bologna, 40129, Italy
SOURCE: Journal of the American Chemical Society (2001), 123(47), 11600-11607
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

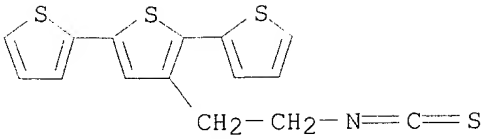
AB The regioselective synthesis of fluorescent oligothiophene isothiocyanates is described. The isothiocyanates were reacted with bovine serum albumin (BSA) following std. procedures and the optical properties of the oligothiophene-BSA **conjugates** were analyzed as a function of oligomer concn., time, and irradn. power. The oligothiophene-BSA **conjugates** were chem. very stable and their photoluminescence characteristics persisted unaltered for several months. Photoluminescence data relative to the **conjugate** of an oligothiophene-S,S-dioxide isothiocyanate with monoclonal anti-CD8 **antibody** are reported. No fluorescence quenching was obsd. following the binding of the isothiocyanate to the **antibody** and the **conjugate** displayed high chem. stability and photostability.

IT **376393-41-8DP**, reaction **conjugated** with bovine serum albumin **385369-25-5DP**, reaction **conjugated** with bovine serum albumin **385369-31-3DP**, reaction **conjugated** with bovine serum albumin **385369-34-6DP**, reaction **conjugated** with CD8 **antibody**
RL: ARU (Analytical role, unclassified); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation)
(oligothiophene isothiocyanates as a new class of **fluorescent markers** for biopolymers)

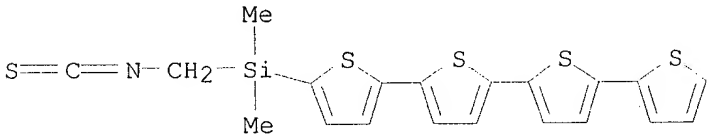
RN 376393-41-8 HCAPLUS
CN 2,2':5',2''-Terthiophene, 5-(2-isothiocyanatoethyl)- (9CI) (CA INDEX NAME)



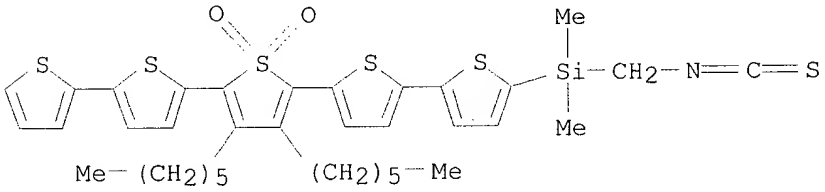
RN 385369-25-5 HCAPLUS
CN 2,2':5',2''-Terthiophene, 3'-(2-isothiocyanatoethyl)- (9CI) (CA INDEX NAME)



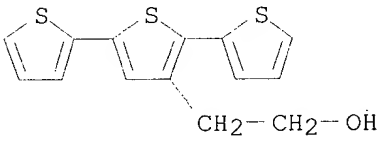
RN 385369-31-3 HCAPLUS
CN Silane, (isothiocyanatomethyl)dimethyl[2,2':5',2'':5'',2'''-quaterthiophen]-5-yl- (9CI) (CA INDEX NAME)



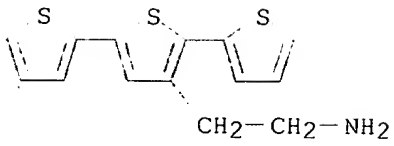
RN 385369-34-6 HCAPLUS
CN Silane, (3'',4''-dihexyl-1'',1''-dioxido[2,2',5':2'':5'',2''':5''',2''''-quinquethiophen]-5-yl)(isothiocyanatomethyl)dimethyl- (9CI) (CA INDEX NAME)



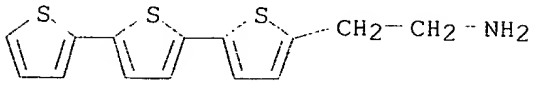
IT **273400-09-2P**, [2,2':5',2''-Terthiophene]-3'-ethanol
385369-23-3P, [2,2':5',2''-Terthiophene]-3'-ethanamine
385369-24-4P, [2,2':5',2''-Terthiophene]-5-ethanamine
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(oligothiophene isothiocyanates as a new class of **fluorescent markers** for biopolymers)
RN 273400-09-2 HCAPLUS
CN [2,2':5',2''-Terthiophene]-3'-ethanol (9CI) (CA INDEX NAME)



RN 385369-23-3 HCAPLUS
CN [2,2':5',2''-Terthiophene]-3'-ethanamine (9CI) (CA INDEX NAME)



RN 385369-24-4 HCAPLUS
CN [2,2':5',2''-Terthiophene]-5-ethanamine (9CI) (CA INDEX NAME)



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ibib abs hitstr 2

L51 ANSWER 2 OF 7 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:699243 HCAPLUS
DOCUMENT NUMBER: 136:32334
TITLE: Direct **DNA** hybridization detection based on the **oligonucleotide**-functionalized conductive polymer
AUTHOR(S): Lee, Tae-Young; Shim, Yoon-Bo
CORPORATE SOURCE: Department of Chemistry, Pusan National University, Keumjeong-ku Pusan, 609-735, S. Korea
SOURCE: Analytical Chemistry (2001), 73(22), 5629-5632
CODEN: ANCHAM; ISSN: 0003-2700
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

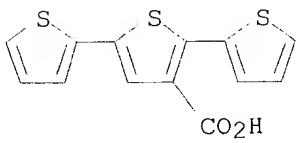
AB Electrochem. methods for **DNA** hybridization detection have many advantages that are very fast to detect hybridization and can be directly applied for a portable **DNA** sensor. In this paper, an electrochem. method to directly detect **DNA** hybridization was developed on the basis of a new conductive polymer, which was polymd. on the glassy carbon electrode with a terthiophene monomer having a carboxyl group (3'-carboxyl-5,2',5',2''-terthiophene). The ss-**DNA** probe was made by chem. bonding an amine-linked C6 alkyl group to the 5' terminus of **oligonucleotide** (19-mer). The probe moiety was immobilized on the polymer through covalent bonding with a catalyst, 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide. A difference in admittance was obsd. before and after hybridization as a result of the redn. of the resistance after hybridization. The highest difference in admittance was obsd. around 1 kHz before and after hybridization. Hybridization amts. of end two-base and center one-base mismatched sequences were obtained only in a 14.3% response when compared to that for the complementary matched sequence.

IT **380630-96-6P**
RL: DEV (Device component use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(direct **DNA** hybridization detection based on **oligonucleotide**-functionalized conductive polymer)

RN 380630-96-6 HCAPLUS
CN [2,2':5',2''-Terthiophene]-3'-carboxylic acid, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 380630-95-5
CMF C13 H8 O2 S3



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ind 2

L51 ANSWER 2 OF 7 HCAPLUS COPYRIGHT 2002 ACS
CC 3-1 (Biochemical Genetics)
Section cross-reference(s): 9
ST **DNA** hybridization detection **oligonucleotide** conductive polymer probe
IT **Nucleic** acid hybridization
(**DNA-DNA**; direct **DNA** hybridization detection based on **oligonucleotide**-functionalized conductive polymer)
IT **Oligonucleotides**
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
(amine-linked C6 alkyl group **conjugates**; direct **DNA** hybridization detection based on **oligonucleotide**-functionalized conductive polymer)
IT Conducting polymers
(direct **DNA** hybridization detection based on **oligonucleotide**-functionalized conductive polymer)
IT Electrodes
(glassy carbon, polymn. on; direct **DNA** hybridization detection based on **oligonucleotide**-functionalized conductive polymer)
IT Electric conductivity
(measurement, and hybridization detection; direct **DNA** hybridization detection based on **oligonucleotide**-functionalized conductive polymer)
IT Probes (**nucleic** acid)
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
(**oligonucleotide** bonding amine-linked C6 alkyl group; direct **DNA** hybridization detection based on **oligonucleotide**-functionalized conductive polymer)
IT Electric resistance
(redn. of, after hybridization; direct **DNA** hybridization detection based on **oligonucleotide**-functionalized conductive polymer)
IT 1892-57-5, 1-Ethyl-3-(3-dimethylaminopropyl)carbodiimide
RL: CAT (Catalyst use); USES (Uses)
(catalyst; direct **DNA** hybridization detection based on **oligonucleotide**-functionalized conductive polymer)
IT **380630-96-6P**
RL: DEV (Device component use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(direct **DNA** hybridization detection based on **oligonucleotide**-functionalized conductive polymer)

=> d ibib abs hitstr 3

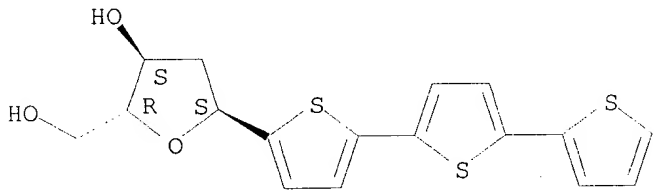
L51 ANSWER 3 OF 7 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:41752 HCAPLUS
DOCUMENT NUMBER: 132:194595
TITLE: Novel nucleoside analogues with fluorophores replacing the **DNA** base
AUTHOR(S): Strassler, Christoph; Davis, Newton E.; Kool, Eric T.
CORPORATE SOURCE: Department of Chemistry, University of Rochester, Rochester, NY, 14627, USA
SOURCE: Helvetica Chimica Acta (1999), 82(12), 2160-2171
CODEN: HCACAV; ISSN: 0018-019X
PUBLISHER: Verlag Helvetica Chimica Acta
DOCUMENT TYPE: Journal
LANGUAGE: English

AB We describe the prepn. and fluorescence properties of a set of new nucleosides in which a known hydrocarbon or oligothiophene fluorophore replaces the **DNA** base at C(1) of the deoxyribose moiety. These compds. are potentially useful as probes in the study of the structure and dynamics of **nucleic** acids and their complexes with **proteins**. In addn., they may find use as fluorescent labels for **nucleic**-acid-based biomedical diagnostics methods. The fluorophores **conjugated** to deoxyribose at C(1) in the .alpha.-D-form include terphenyl, stilbene, terthiophene, benzoterthiophene, and pyrene. Also included is a non-fluorescent spacer in which cyclohexene replaces the **DNA** base. The nucleosides are derived from brominated fluorophore precursors and Hoffer's 2-deoxy-3,5-di-O-(p-toluoyl)-D-ribofuranosyl chloride. The emission maxima of the free nucleosides range from 345 to 536 nm. Also described are the 5'-(dimethoxytrityl) 3'-O-phosphoramidite derivs. suitable for incorporation into **oligonucleotides** by automated synthesizers.

IT **259801-06-4P 259801-07-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of novel nucleoside analogs with fluorophores replacing the **DNA** base)

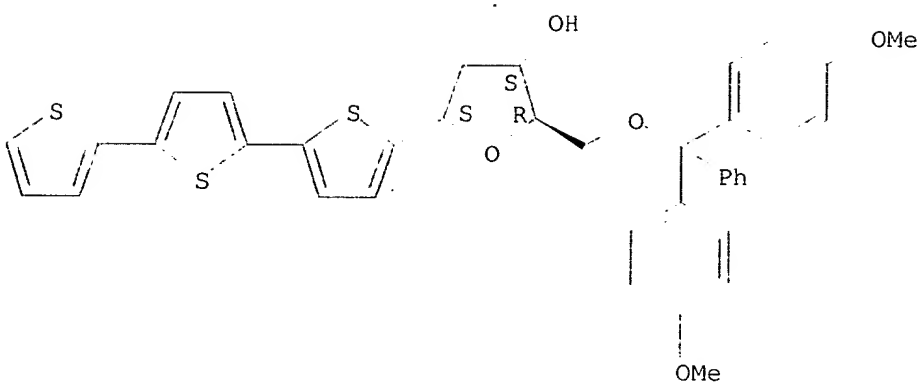
RN 259801-06-4 HCAPLUS
CN D-erythro-Pentitol, 1,4-anhydro-2-deoxy-1-C-[2,2':5',2''-terthiophen]-5-yl-, (1S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 259801-07-5 HCAPLUS
CN D-erythro-Pentitol, 1,4-anhydro-5-O-[bis(4-methoxyphenyl)phenylmethyl]-2-deoxy-1-C-[2,2':5',2''-terthiophen]-5-yl-, (1S)- (9CI) (CA INDEX NAME)

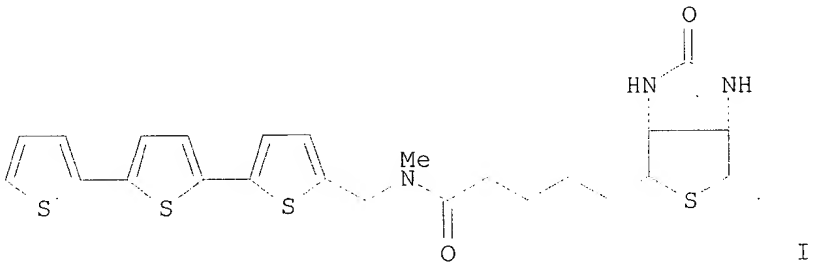
Absolute stereochemistry.



REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ibib abs hitstr 4

L51 ANSWER 4 OF 7 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1996:528314 HCAPLUS
DOCUMENT NUMBER: 125:300730
TITLE: A new synthetic route to 2,2':5',2''-terthiophene-5-derivatives to **conjugate** with **proteins** and monoclonal **antibodies**
AUTHOR(S): Cosimelli, Barbara; Neri, Dario; Roncucci, Gabrio
CORPORATE SOURCE: Molteni Farmaceutici, Florence, Italy
SOURCE: Tetrahedron (1996), 52(34), 11281-11290
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

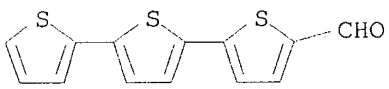


I

AB A no. of terthiophene derivs. which can be linked to **proteins** or other carrier mols. by using different functional groups were synthesized and characterized. The **conjugation** of some of these compds. to carrier **proteins** and **antibodies** was described. An example compd. is the N-[(terthienyl)methyl]biotinpentanamide **conjugate** I. The possible applications of I as photosensitizer were discussed (no data).

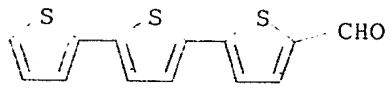
IT **7342-41-8DP**, [2,2':5',2''-Terthiophene]-5-carboxaldehyde, **conjugates** with **proteins** or **antibodies**
RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
(prepn. of terthiophene **conjugates** with **proteins** or **antibodies**)

RN 7342-41-8 HCAPLUS
CN [2,2':5',2''-Terthiophene]-5-carboxaldehyde (7CI, 8CI, 9CI) (CA INDEX NAME)



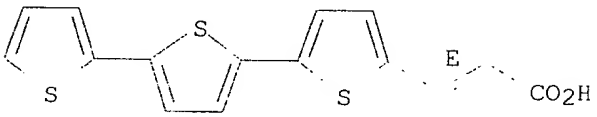
IT **7342-41-8**, [2,2':5',2''-Terthiophene]-5-carboxaldehyde
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of terthiophene **conjugates** with **proteins** or **antibodies**)

RN 7342-41-8 HCAPLUS
CN [2,2':5',2''-Terthiophene]-5-carboxaldehyde (7CI, 8CI, 9CI) (CA INDEX NAME)



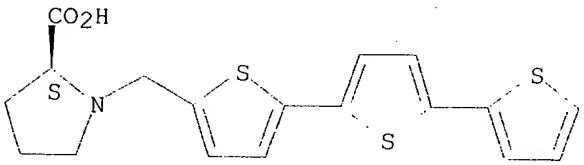
IT **137584-58-8P 174563-35-0P 174563-36-1P**
174563-40-7P 182629-28-3P 182629-31-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of terthiophene **conjugates** with **proteins** or **antibodies**)
RN 137584-58-8 HCAPLUS
CN 2-Propenoic acid, 3-[2,2':5',2''-terthiophen]-5-yl-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

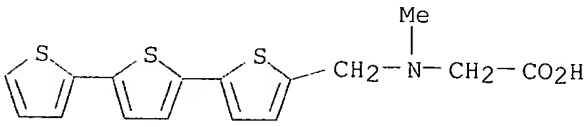


RN 174563-35-0 HCAPLUS
CN L-Proline, N-([2,2':5',2''-terthiophen]-5-ylmethyl)- (9CI) (CA INDEX NAME)

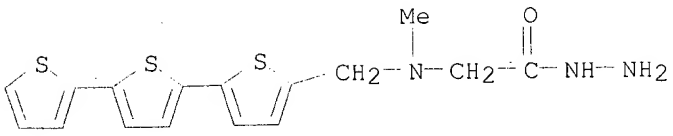
Absolute stereochemistry.



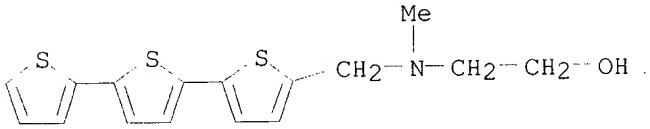
RN 174563-36-1 HCAPLUS
CN Glycine, N-methyl-N-([2,2':5',2''-terthiophen]-5-ylmethyl)- (9CI) (CA INDEX NAME)



RN 174563-40-7 HCAPLUS
CN Glycine, N-methyl-N-([2,2':5',2''-terthiophen]-5-ylmethyl)-, hydrazide (9CI) (CA INDEX NAME)

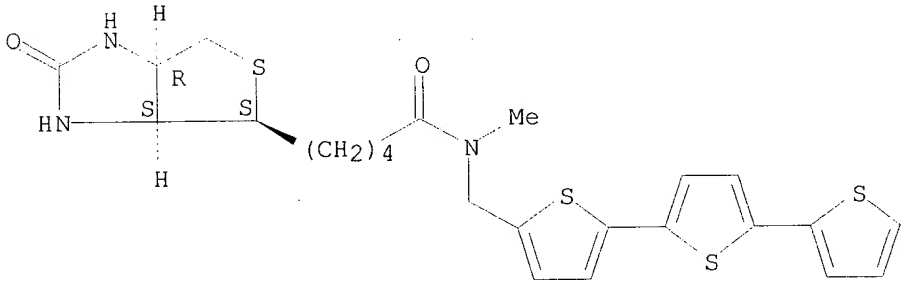


RN 182629-28-3 HCAPLUS
CN Ethanol, 2-[methyl([2,2':5',2''-terthiophen]-5-ylmethyl)amino]- (9CI) (CA INDEX NAME)



RN 182629-31-8 HCAPLUS
CN 1H-Thieno[3,4-d]imidazole-4-pentanamide, hexahydro-N-methyl-2-oxo-N-([2,2':5',2''-terthiophen]-5-ylmethyl)-, [3aS-(3a.alpha.,4.beta.,6a.alpha.)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> d ibib abs hitstr 5

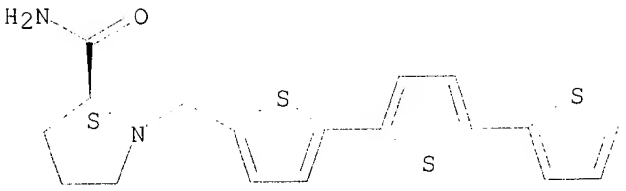
L51 ANSWER 5 OF 7 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1996:418719 HCAPLUS
DOCUMENT NUMBER: 125:109072
TITLE: Targeted photolysis of melanoma cells by using an alpha-terthienyl derivative labeled anti-melanoma monoclonal **antibody**
AUTHOR(S): Roncucci, G.; Stefano, A. Di; Soldani, P.; Neri, P.; Neri, D.
CORPORATE SOURCE: Molteni Farmaceutici, Scandicci, 50018, Italy
SOURCE: Proceedings of SPIE-The International Society for Optical Engineering (1996), 2625(Photochemistry: Photodynamic Therapy and Other Modalities), 550-560
CODEN: PSISDG; ISSN: 0277-786X
PUBLISHER: SPIE-The International Society for Optical Engineering
DOCUMENT TYPE: Journal
LANGUAGE: English

AB **Antibody** targeted chemotherapy is a relatively new technique which involves the specifically carrier mediated delivery of chemotherapeutic agents to tumors or other pathogens for the treatment of such deseases. **Conjugation** of **antibodies** with photosensitizers (PSs) can also lead to potential therapeutic agents which combine photodynamic cytotoxicity with specific **antibody** binding. The **antibody** mediated delivery of a photosensitizer mol. and the target destruction upon irradn. by light followed by prodn. of singlet oxygen or other radicals, results in a higher therapeutic ratio compared to the conventional photodynamic therapy (PDT). In this study the naturally occurring PS .alpha.-terthienyl (ATT) was chem. derivatized with an amino group specific reactive side arm and to exploit its toxicity as an effector function suitable for targeted photolysis, covalently **conjugated** to the 225.28S monoclonal **antibody** (mAb) specific for the high mol. wt. melanoma assocd. antigen (HMW-MAA). The 225-28S-ATT **conjugate** prepd. was then tested against the melanoma cell line Colo38 in comparison with HT29 tumor cells, not recognized by 225-28S mAb, as neg. control. The selective uptake of labeled mAb 225-28S-ATT was obsd. and melanoma cell death following irradn. occurred. In conclusion the 225-28S-ATT **conjugate**, as far as one can judge from the effect on cells grown in vitro, seems a good candidate as a model to test the **antibody** targeted photolysis of melanoma cells for developing specific antimelanoma therapeutic agents.

IT **179339-14-1D**, monoclonal **antibody conjugates**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(targeted photolysis of melanoma cells by .alpha.-terthienyl deriv. labeled anti-melanoma monoclonal **antibody**)

RN 179339-14-1 HCAPLUS
CN 2-Pyrrolidinecarboxamide, 1-([2,2':5',2''-terthiophen]-5-ylmethyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.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N
S
S
S

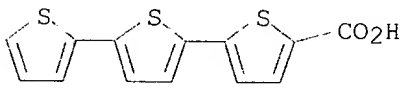
=> d ibib abs hitstr 6

L51 ANSWER 6 OF 7 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1996:398994 HCAPLUS
DOCUMENT NUMBER: 125:80576
TITLE: Study of photoinduced energy and electron transfer in .alpha.-terthienyl-bovine serum albumin **conjugates**: a laser flash photolysis study
AUTHOR(S): Boch, R.; Mohtat, N.; Lear, Y.; Arnason, J. T.; Durst, T.; Scaiano, J. C.
CORPORATE SOURCE: Dep. CHem. Biol., Univ. Ottawa, Ottawa, Can.
SOURCE: Photochemistry and Photobiology (1996), 64(1), 92-99
CODEN: PHCBAP; ISSN: 0031-8655
PUBLISHER: American Society for Photobiology
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The photochem. of .alpha.-terthienyl (.alpha.-T) has been examd. in bovine serum albumin (BSA). Freely assocd. and covalently **conjugated** .alpha.-T chromophores show similar behavior toward nonpolar quenchers such as oxygen and benzoquinone but show significant differences in the case of quenching by Me viologen, a water-sol. cationic electron acceptor; in this case, triplet quenching reveals two distinct .alpha.-T populations, attributed to chromophores in sites showing very different accessibility from the aq. phase. Rate consts. for triplet quenching in BSA are generally slower than thos obsd. in homogeneous soln. for free .alpha.-T. For examples, in the case of oxygen, the rate const. is about one order of magnitude smaller when .alpha.-T is assocd. or **conjugated** with the **protein** compared with .alpha.-T in soln. While triplet yields for .alpha.-T are essentially the same in soln. and in the **protein** environment, the yield of detectable singlet oxygen is substantially reduced in the **protein**. This is attributed to a geminate reaction within the **protein** involving singlet oxygen trapping in the vicinity of the generation site.

IT **87145-85-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; photoinduced energy and electron transfer in .alpha.-terthienyl-bovine serum albumin **conjugates**: laser flash photolysis study)

RN 87145-85-5 HCAPLUS
CN [2,2':5',2''-Terthiophene]-5-carboxylic acid (9CI) (CA INDEX NAME)



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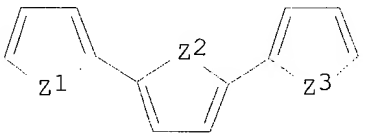
L51 ANSWER 7 OF 7 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1996:171806 HCAPLUS
DOCUMENT NUMBER: 124:232237
TITLE: Preparation of photodynamic .alpha.-terthiophene **conjugates** with biocidal properties
INVENTOR(S): Neri, Giovanni; Roncucci, Gabrio
PATENT ASSIGNEE(S): L. Molteni e C. dei Fratelli Alitti Societa' di Esercizio Societa' per Azioni, Italy
SOURCE: PCT Int. Appl., 37 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9532001	A1	19951130	WO 1995-EP1938	19950522
W: AM, AU, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LV, MD, MG, MN, MW, MX, NO, NZ, PL, RO, RU, SD, SG, SI, SK, TJ, TM, TT, UA, US, UZ, VN				
RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2191195	AA	19951130	CA 1995-2191195	19950522
AU 9525662	A1	19951218	AU 1995-25662	19950522
EP 760679	A1	19970312	EP 1995-920073	19950522
EP 760679	B1	20000419		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, NL, PT, SE				
AT 191852	E	20000515	AT 1995-920073	19950522
ES 2147288	T3	20000901	ES 1995-920073	19950522
US 5869051	A	19990209	US 1996-750021	19961122

PRIORITY APPLN. INFO.: IT 1994-FI95 A 19940523
WO 1995-EP1938 W 19950522
OTHER SOURCE(S): MARPAT 124:232237
GI



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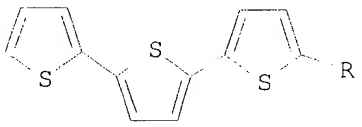
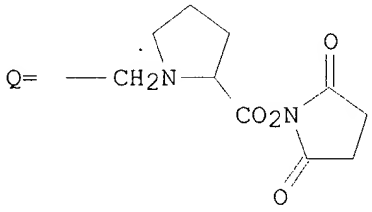


II

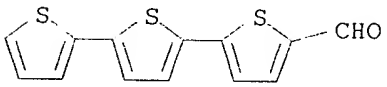


AB Photodyn. **conjugates** consisting of a carrier mol. and of an org. mol., preferably terthiophene or analogs (I; Z1 - Z3 = S, O), able to

efficiently produce singlet oxygen after irradn. are prepd. I is suitably derivatized in order to react with an amino, thiol saccharide, histidine, and tyrosine group of the carrier mol. Said carrier mols. are selected from **antibodies**, peptides, heptamers, sugars, or other analogous carriers able to direct the photosensitizer mol. toward a biol. target, e.g. Con A, avidin, biotin, monoclonal **antibody**-anti-Candida albicans, monoclonal **antibody** anti-Herpes simplex virus 1 or 2, and monoclonal **antibody** anti-Rubella virus. Said **conjugates** (e.g. .alpha.-terthiophene **conjugates** with Con A, avidin, biotin, monoclonal **antibody**-anti-Candida albicans, monoclonal **antibody** anti-Herpes simplex virus 1 or 2, and monoclonal **antibody** anti-Rubella virus) are useful either for therapeutic or diagnostic purposes, e.g., as antibacterial, antiviral, antifungal, and antitumor agents. Thus, formylation of 2,2':5',2''-terthiophene (II; R = H) by N-methylformanilide and POCl3 in CH2Cl2 under reflux for 40 h to 5-formyl-.alpha.-terthiophene II (R = CHO) followed reductive alkylation with proline in the presence of NaBH4 and mol. sieves in MeOH at room temp. for 12 h gave the N-(terthiophenylmethyl)L-proline II (R = CH2-Pro-OH), which was esterified with N-hydroxysuccinimide using DCC in DMF/CH2Cl2 at room temp. for 20 h to give the active ester II (R = Q). The latter compd. was coupled with Con A (ConA) in 100 mM phosphate buffer (pH 8) to give the ConA-.alpha.-terthiophene **conjugate**. Suspension of Candida albicans and Saccharomyces cerevisiae was incubated in the dark with the latter **conjugate** at 3 .times. 10-8 M for 0.5 h and then irradiated at 350 nm for 30 min and incubated in the dark for 24 h at 33.degree.. The growth of the treated fungi was completely inhibited. Monoclonal **antibodies** against Herpes simplex virus 1 or 2, Candida albicans, anti-Rubella virus, and 225-28S.

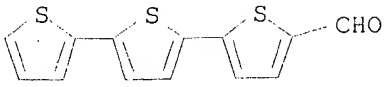
IT **7342-41-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(antibacterial agent by itself; prepn. of photodynamic .alpha.-terthiophene **conjugates** for producing singlet oxygen as biocides or diagnostics)

RN 7342-41-8 HCAPLUS
CN [2,2':5',2''-Terthiophene]-5-carboxaldehyde (7CI, 8CI, 9CI) (CA INDEX NAME)



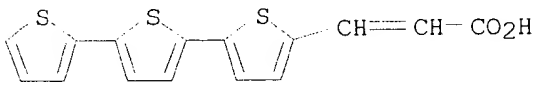
IT **7342-41-8DP, conjugates** with bovine serum albumin
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of photodynamic .alpha.-terthiophene **conjugates** for producing singlet oxygen as biocides or diagnostics)

RN 7342-41-8 HCAPLUS
CN [2,2':5',2''-Terthiophene]-5-carboxaldehyde (7CI, 8CI, 9CI) (CA INDEX NAME)



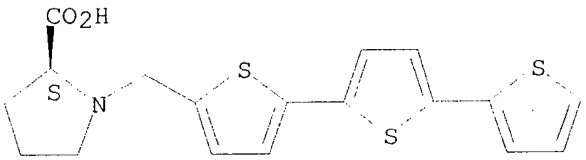
IT **138024-51-8P 174563-35-0P 174563-36-1P**
174563-40-7P 174563-42-9P 174563-43-0P
174563-47-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of photodynamic .alpha.-terthiophene **conjugates** for producing singlet oxygen as biocides or diagnostics)

RN 138024-51-8 HCAPLUS
CN 2-Propenoic acid, 3-[2,2':5',2''-terthiophen]-5-yl- (9CI) (CA INDEX NAME)

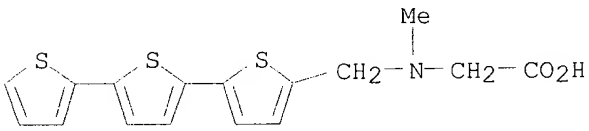


RN 174563-35-0 HCAPLUS
CN L-Proline, N-([2,2':5',2''-terthiophen]-5-ylmethyl)- (9CI) (CA INDEX NAME)

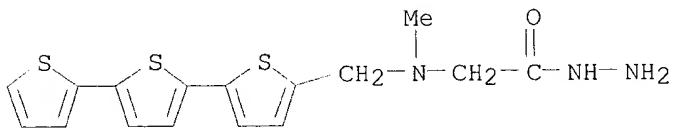
Absolute stereochemistry.



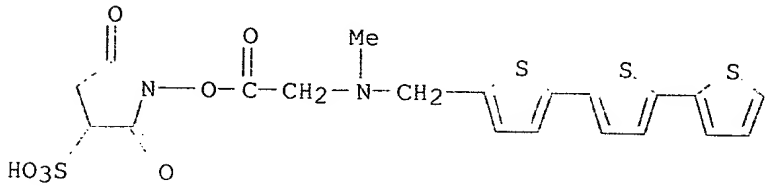
RN 174563-36-1 HCAPLUS
CN Glycine, N-methyl-N-([2,2':5',2''-terthiophen]-5-ylmethyl)- (9CI) (CA INDEX NAME)



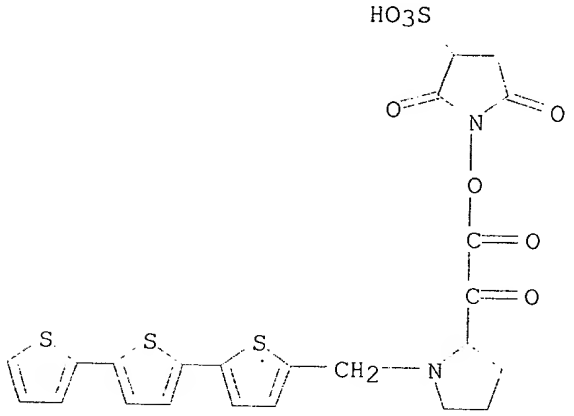
RN 174563-40-7 HCAPLUS
CN Glycine, N-methyl-N-([2,2':5',2''-terthiophen]-5-ylmethyl)-, hydrazide (9CI) (CA INDEX NAME)



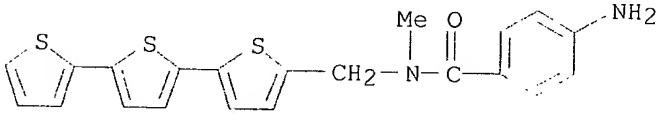
RN 174563-42-9 HCAPLUS
CN 3-Pyrrolidinesulfonic acid, 1-[[[methyl([2,2':5',2''-terthiophen]-5-ylmethyl)amino]acetyl]oxy]-2,5-dioxo- (9CI) (CA INDEX NAME)



RN 174563-43-0 HCAPLUS
CN 3-Pyrrolidinesulfonic acid, 2,5-dioxo-1-[[oxo[1-([2,2':5',2''-terthiophen]-5-ylmethyl)-2-pyrrolidinyl]acetyl]oxy]- (9CI) (CA INDEX NAME)



RN 174563-47-4 HCAPLUS
CN Benzamide, 4-amino-N-methyl-N-([2,2':5',2''-terthiophen]-5-ylmethyl)- (9CI) (CA INDEX NAME)



for explanation of this d que see L51 query display

TRAN 09/871,353

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                 OR L6 OR L7 OR L8)
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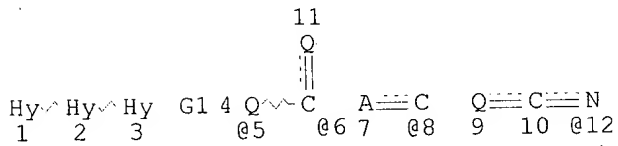


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DEFAULT ECLEVEL IS LIMITED
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ECOUNT  IS E4 C  E1 S  AT   2
ECOUNT  IS E4 C  E1 S  AT   3

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  12

STEREO ATTRIBUTES: NONE
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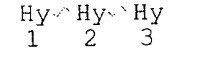


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Searched by Susan Hanley 305-4053

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ECOUNT  IS E4 C  E1 S  AT   3

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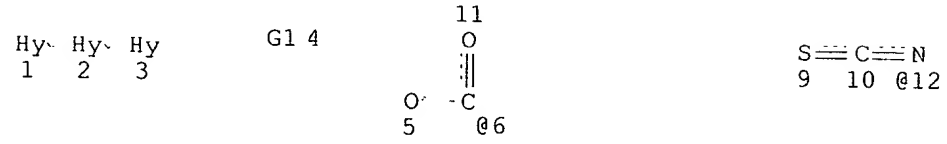

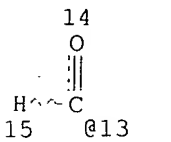


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GGCAT   IS MCY  UNS  AT   2
GGCAT   IS MCY  UNS  AT   3
DEFAULT ECLEVEL IS LIMITED
ECOUNT  IS E4 C  E1 S  AT   1
ECOUNT  IS E4 C  E1 S  AT   2
ECOUNT  IS E4 C  E1 S  AT   3

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  13

STEREO ATTRIBUTES: NONE
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L30          104 SEA FILE=REGISTRY ABB=ON  PLU=ON  L27 AND  5 16.145.3/RID
L31          746 SEA FILE=REGISTRY ABB=ON  PLU=ON  (L28 OR L29 OR L30)
L32          674 SEA FILE=REGISTRY ABB=ON  PLU=ON  L31 AND NC=1 NOT ("DIAZO" OR
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L33        23948 SEA FILE=REGISTRY ABB=ON  PLU=ON  2 16.145.3/RID
L35         2996 SEA FILE=REGISTRY ABB=ON  PLU=ON  L33 AND "BITHIOPHENE"
L38          662 SEA FILE=REGISTRY ABB=ON  PLU=ON  L35 AND ("HYDROXY" OR
                 "HYDROXYL" OR "CARBOXALDEHYDE" OR "FORMYL" OR  "ISOTHIOCYANATO"
                  OR "THIOL" OR "AMINO" OR "CARBOXYLIC") NOT "ESTER"
L39          584 SEA FILE=REGISTRY ABB=ON  PLU=ON  L38 AND NC=1
L40          451 SEA FILE=REGISTRY ABB=ON  PLU=ON  L39 NOT "AZO"
L41          287 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L32
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TRAN 09/871,353

L42	455	SEA FILE=HCAPLUS ABB=ON PLU=ON L40
L43	15	SEA FILE=HCAPLUS ABB=ON PLU=ON L41(L)?CONJUGAT?
L44	14	SEA FILE=HCAPLUS ABB=ON PLU=ON L42(L)?CONJUGAT?
L45	26	SEA FILE=HCAPLUS ABB=ON PLU=ON L43 OR L44
L46	25	SEA FILE=HCAPLUS ABB=ON PLU=ON L45 NOT L15
L47	3042811	SEA FILE=HCAPLUS ABB=ON PLU=ON ANTIBOD? OR FLUORESC?(3A)MARKER OR PROTEIN OR DNA OR NUCLEIC OR OLIGONUC? OR HORMON? OR DRUG OR MEDICINE OR NEUROTRANSMITTER
L48	121828	SEA FILE=HCAPLUS ABB=ON PLU=ON SPECTROFLUORIMETRY OR CYTOMETRY OR FLUORESCENCE(W)MICROSCO? OR GEL ELECTROPHOR?
L49	40	SEA FILE=HCAPLUS ABB=ON PLU=ON (L41 OR L42) AND (L47 OR L48)
L50	8	SEA FILE=HCAPLUS ABB=ON PLU=ON L49 AND ?CONJUGAT?
L51	7	SEA FILE=HCAPLUS ABB=ON PLU=ON L50 NOT L15
L52	20	SEA FILE=HCAPLUS ABB=ON PLU=ON L46 NOT L51
L53	18	SEA FILE=HCAPLUS ABB=ON PLU=ON L52 NOT PATENT/DT
L54	17	SEA FILE=HCAPLUS ABB=ON PLU=ON L53 AND PD<20010530
L55	4	SEA FILE=HCAPLUS ABB=ON PLU=ON L54 AND (VISIBLE(3A)(UV OR ULTRAVIOET))

4 cites

Searched by Susan Hanley 305-4053

=> d ibib abs hitstr 1

L55 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:527050 HCAPLUS
DOCUMENT NUMBER: 135:288881
TITLE: Synthesis, structures and nonlinear optical properties of novel D-.pi.-A chromophores: intramolecular charge transfer from 1,3-dithiole or ferrocene moieties to polynitrofluorene or dicyanomethylene moieties through conjugated linkers
AUTHOR(S): Moore, Adrian J.; Chesney, Antony; Bryce, Martin R.; Batsanov, Andrei S.; Kelly, Janet F.; Howard, Judith A. K.; Perepichka, Igor F.; Perepichka, Dmitrii F.; Meshulam, Guilia; Berkovic, Garry; Kotler, Zvi; Mazor, Royi; Khodorkovsky, Vladimir
CORPORATE SOURCE: Department of Chemistry, University of Durham, Durham, DH1 3LE, UK
SOURCE: European Journal of Organic Chemistry (2001), (14), 2671-2687
CODEN: EJOCFK; ISSN: 1434-193X
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:288881
GI

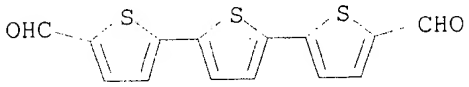
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Electron donor-.pi.-acceptor chromophores, e.g., I (R = MeS) and II (R = NO2 (38a), CO2Me (38b), CO2(CH2CH2O)3Me (38c), Fc = ferrocenyl), were synthesized. The donor units are 1,3-dithiole and ferrocene; conjugated ethylenic, Ph, phenylenevinylene, thienyl, bithienyl, terthienyl, or thienylenevinylene linkers act as a central .pi.-electron relay unit, and dicyanomethylene and polynitrofluorene groups as the acceptor unit. The electronic absorption spectra display a broad low-energy intramol. charge transfer band in the visible region (500-700 nm) the energy (hvICT .apprxeq. 1.7-2.5 eV) and intensity (.epsilon. .apprxeq. 5000-50000 m-1cm-1) of which depend substantially on the nature of both D and A moieties and on the structure of the linker unit. Nonlinear optical properties were evaluated using the EFISH technique: the highest .mu..beta.(0) values are obsd. for 38b [(900 .+-. 300).times.10-48 esu] and 42 (shown as III) [(1800 .+-. 300).times.10-48 esu] establishing that polynitrofluorene is a promising acceptor terminal moiety in this context. The mol. and electronic structures of 49 and 50 (shown as IV and I (R = H), resp.) were calcd. by the RHF/6-31G(d)//RHF/6-31G(d) ab initio method. The HOMO is located mostly in the 1,3-dithiolium ring, and the LUMO mostly at the dicyanomethylene fragment (and the Ph ring of 50) although the electronic population at C2 of the 1,3-dithiolium rings is also considerable. The x-ray crystal structures of 9, 18 (shown as V and VI, resp.), and (E)-p-[(NC)2C:CH]C6H4CH:CHFc (27), were reported. In all three structures the conjugated .pi.-systems are effectively planar with extensive .pi.-electron delocalization between the donor and acceptor moieties. The planar conformation of 18 gives rise to a close intramol. S-S contact of 3.095(3) .ANG. between the dithiole and thiophene units.

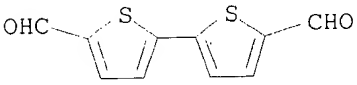
IT **13130-50-2 32364-72-0**, 2,2'-Bithiophene-5,5'-dialdehyde
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. and nonlinear optical properties of D-.pi.-A chromophores from

1,3-dithiole or ferrocene moieties contg. polynitrofluorene or dicyanomethylene moieties through **conjugated** linkers)

RN 13130-50-2 HCAPLUS
CN [2,2':5',2''-Terthiophene]-5,5''-dicarboxaldehyde (8CI, 9CI) (CA INDEX NAME)

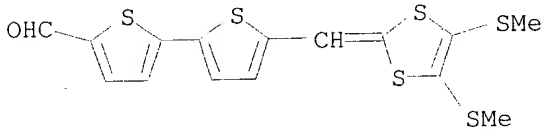


RN 32364-72-0 HCAPLUS
CN [2,2'-Bithiophene]-5,5'-dicarboxaldehyde (7CI, 8CI, 9CI) (CA INDEX NAME)

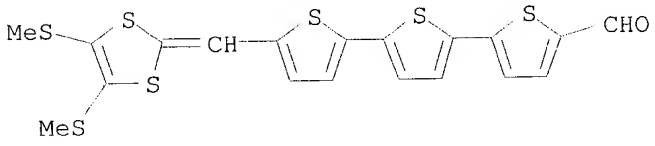


IT **365210-82-8P 365210-83-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and nonlinear optical properties of D-.pi.-A chromophores from 1,3-dithiole or ferrocene moieties contg. polynitrofluorene or dicyanomethylene moieties through **conjugated** linkers)

RN 365210-82-8 HCAPLUS
CN [2,2'-Bithiophene]-5-carboxaldehyde, 5'-[[4,5-bis(methylthio)-1,3-dithiol-2-ylidene]methyl]- (9CI) (CA INDEX NAME)



RN 365210-83-9 HCAPLUS
CN [2,2':5',2''-Terthiophene]-5-carboxaldehyde, 5''-[[4,5-bis(methylthio)-1,3-dithiol-2-ylidene]methyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 109 THERE ARE 109 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ind

L55 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2002 ACS
CC 29-12 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 25, 27, 28, 73, 75

ST crystal structure ferrocene thiophene phenylene thiophenylene dicyanomethylene deriv; nonlinear optical property dithiole ferrocene polynitrofluorene dicyanomethylene deriv prepn; electronic structure dithiolylidene dicyanomethylene deriv; HOMO LUMO dithiolylidene dicyanomethylene deriv; mol structure ferrocene thiophene phenylene thiophenylene dicyanomethylene deriv; charge transfer intramol dithiole ferrocene polynitrofluorene dicyanomethylene deriv; RHF MO calcn dithiolylidene dicyanomethylene deriv; safety exothermic reaction ferrocenylpentadienal prepn

IT Electron delocalization
(between donor and acceptor moieties in dithiolylidene and dicyanomethylene-contg. model electron donor-.pi.-acceptor moieties)

IT Safety
(hazard due to exothermic reaction during prepn. ferrocenylpentadienal as intermediate in prepn. of D-.pi.-A chromophore contg. ferrocene and dicyano moieties)

IT Electron transfer
(intramol.; synthesis, structures and nonlinear optical properties of novel D-.pi.-A chromophores and intramol. charge transfer from 1,3-dithiole or ferrocene moieties to polynitrofluorene or dicyanomethylene moieties through conjugated linkers)

IT HOMO (molecular orbital)
LUMO (molecular orbital)
RHF (molecular orbital)
(of dithiolylidene and dicyanomethylene-contg. model electron donor-.pi.-acceptor model chromophores)

IT Electronic structure
Second-order nonlinear optical properties
UV and **visible** spectra
(of electron donor-.pi.-acceptor chromophores contg. dithiole, ferrocene, polynitrofluorene, and dicyanomethylene moieties)

IT Crystal structure
Molecular structure
(of ferrocene- and dithiole-contg. chromophores contg. phenylene or thiophenylene and dicyanomethylene moieties)

IT Molecular orbital
(optimized; of dithiolylidene and dicyanomethylene-contg. model electron donor-.pi.-acceptor model chromophores)

IT Chromophores
(synthesis, structures and nonlinear optical properties of novel D-.pi.-A chromophores and intramol. charge transfer from 1,3-dithiole or ferrocene moieties to polynitrofluorene or dicyanomethylene moieties through conjugated linkers)

IT 365210-95-3 365210-96-4
RL: PRP (Properties)
(electronic and mol. structures calcd. by RHF ab initio method)

IT 223134-50-7P 241161-37-5P 241161-39-7P 241161-47-7P 365210-81-7P
365210-84-0P 365210-85-1P 365210-86-2P 365210-87-3P 365210-88-4P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and electronic absorption spectra of)

IT 241161-53-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and electronic absorption spectra of)

IT 365210-94-2P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and nonlinear optical properties of)

IT 329246-94-8P 329247-02-1P
RL: PRP (Properties); PUR (Purification or recovery); SPN (Synthetic

preparation); PREP (Preparation)
(prepn. and nonlinear optical properties of D-.pi.-A chromophores from 1,3-dithiole or ferrocene moieties contg. polynitrofluorene or dicyanomethylene moieties through conjugated linkers)

IT 109-77-3P, Malononitrile 300710-65-0P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and nonlinear optical properties of D-.pi.-A chromophores from 1,3-dithiole or ferrocene moieties contg. polynitrofluorene or dicyanomethylene moieties through conjugated linkers)

IT 98243-44-8P
RL: PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and nonlinear optical properties of D-.pi.-A chromophores from 1,3-dithiole or ferrocene moieties contg. polynitrofluorene or dicyanomethylene moieties through conjugated linkers)

IT 623-27-8, 1,4-Benzenedicarboxaldehyde 932-95-6, 2,5-Thiophenedicarbaldehyde 1271-47-2, Ferrocenylethyne 12093-10-6, Ferrocenecarboxaldehyde **13130-50-2** 20430-33-5, (4-Cyanobenzyl)triphenylphosphonium chloride 22411-59-2, p-(Diethylamino)cinnamaldehyde **32364-72-0**, 2,2'-Bithiophene-5,5'-dialdehyde 32914-67-3, (Ferrocenylmethyl)triphenylphosphonium iodide 56637-71-9 185426-82-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. and nonlinear optical properties of D-.pi.-A chromophores from 1,3-dithiole or ferrocene moieties contg. polynitrofluorene or dicyanomethylene moieties through **conjugated** linkers)

IT 98243-45-9P 123931-08-8P 183384-17-0P 223134-46-1P 365210-76-0P 365210-78-2P 365210-79-3P **365210-82-8P 365210-83-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and nonlinear optical properties of D-.pi.-A chromophores from 1,3-dithiole or ferrocene moieties contg. polynitrofluorene or dicyanomethylene moieties through **conjugated** linkers)

IT 29210-71-7, 2,4,5,7-Tetranitrofluorene 164297-32-9, 2,5,7-Trinitro-4-methoxycarbonylfluorene 226419-15-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. and nonlinear optical properties of D-.pi.-A electron chromophores from 1,3-dithiole or ferrocene moieties contg. polynitrofluorene or dicyanomethylene moieties through conjugated linkers)

IT 123931-07-7P
RL: BYP (Byproduct); REM (Removal or disposal); PREP (Preparation); PROC (Process)
(prepn. of)

IT 365210-90-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

IT 241161-50-2P 241161-57-9P 241161-58-0P 365210-77-1P 365210-89-5P 365210-92-0P 365210-93-1P 365210-97-5P 365210-98-6P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn., electronic absorption spectra, and nonlinear optical properties of)

IT 196696-74-9P 223134-55-2P 365210-80-6P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn., electronic absorption spectra, nonlinear optical properties, and crystal structure of)

IT 1271-67-6P, Ferrocenyl(formyl)acetylene
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn., reaction with fluorene deriv., and electronic absorption

spectra of)

IT 1272-17-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn.and caution due to exothermic reaction during prepn. as intermediate in prepn. of D-.pi.-A chromophore contg. ferrocene and dicyano moieties)

IT 365210-91-9P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(prepn.and electronic absorption spectra of)

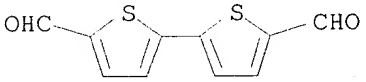
=> d ibib abs hitstr 2

L55 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:498564 HCAPLUS
DOCUMENT NUMBER: 133:252378
TITLE: Mixed .pi.-conjugated oligomers of thiophene and 3,4-ethylenedioxythiophene (EDOT)
AUTHOR(S): Turbiez, M.; Frere, P.; Blanchard, P.; Roncali, J.
CORPORATE SOURCE: Ingenierie Moleculaire et Materiaux Organiques, UMR-CNRS 6501, Angers, 49045, Fr.
SOURCE: Tetrahedron Letters (**2000**), 41(29), 5521-5525
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:252378

AB Conjugated oligomers based on various combinations of thiophene and 3,4-ethylenedioxythiophene (EDOT) moieties were synthesized. Comparison of the optical and electrochem. properties shows that the introduction of a bis-EDOT core in the middle of the system produces a decrease of the HOMO-LUMO gap which is attributed to an enhancement of the planarity and rigidity of the .pi.-conjugated system.

IT **32364-72-0**, 2,2'-Bithiophene-5,5'-dicarboxaldehyde
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of mixed **conjugated** oligomers of thiophene and ethylenedioxythiophene)

RN 32364-72-0 HCAPLUS
CN [2,2'-Bithiophene]-5,5'-dicarboxaldehyde (7CI, 8CI, 9CI) (CA INDEX NAME)



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ind 2

L55 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2002 ACS
CC 28-11 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 22
ST conjugated thiophene oligomer prepn electronic property; oxidn potential UV conjugated thiophene oligomer
IT Oxidation potential
UV and **visible** spectra
(of mixed conjugated oligomers of thiophene and ethylenedioxythiophene)
IT 250726-94-4P 250726-96-6P 295358-38-2P 295358-39-3P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(oxidn. potential and UV spectra)
IT 1003-09-4, 2-Bromothiophene 4805-22-5, 5,5'-Dibromo-2,2'-bithiophene **32364-72-0**, 2,2'-Bithiophene-5,5'-dicarboxaldehyde 126213-50-1 175922-79-9 195602-17-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of mixed **conjugated** oligomers of thiophene and ethylenedioxythiophene)

IT 98-03-3P, 2-Thienaldehyde 199168-63-3P 295358-40-6P 295358-41-7P 295358-42-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of mixed conjugated oligomers of thiophene and ethylenedioxythiophene)

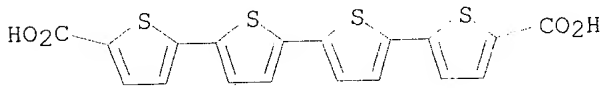
=> d ibib abs hitstr 3

L55 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:457921 HCAPLUS
DOCUMENT NUMBER: 133:193729
TITLE: Redox States of Well-Defined .pi.-Conjugated Oligothiophenes Functionalized with Poly(benzyl ether) Dendrons
AUTHOR(S): Apperloo, Joke J.; Janssen, Rene A. J.; Malenfant, Patrick R. L.; Groenendaal, Lambertus; Frechet, Jean M. J.
CORPORATE SOURCE: Laboratory for Macromolecular and Organic Chemistry, Eindhoven University of Technology, Eindhoven, 5600 MB, Neth.
SOURCE: Journal of the American Chemical Society (**2000**), 122(29), 7042-7051
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The redox states of a series of well-defined hybrid dendrimers based on oligothiophene cores and poly(benzyl ether) dendrons have been studied using cyclic voltammetry and variable-temp. **UV/visible** /near-IR spectroscopy. The oxidn. potentials and the electronic transitions of the neutral, singly oxidized, and doubly oxidized states of these novel hybrid materials have been detd. as a function of oligothiophene conjugation length varying between 4 and 17 repeat units. The attachment of poly(benzyl ether) dendritic wedges at the termini of these lengthy oligothiophenes considerably enhances their soly., thus enabling the first detailed investigation of the electronic structure of oligothiophenes having 11 and 17 repeat units with minimal .beta.-substitution. In the case of the undecamer and heptadecamer, we find that the dicationic state consists of two individual polarons, rather than a single bipolaron. The effect of the dendritic poly(benzyl ether) solubilizers on the properties of the redox states varies with the oligothiophene length and dendron size. More specifically, we observe a kinetic limit to the electrochem. oxidn. of the oligothiophene core when the dendron is large compared to the electrophore. Finally, we have obsd. the first example of self-complexation of cation radicals via .pi.-dimerization leading to the formation of dendritic supramol. assemblies.

IT **288861-01-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(redox states of .pi.-**conjugated** oligothiophenes functionalized with poly(benzyl ether) dendrons)

RN 288861-01-8 HCAPLUS
CN [2,2':5',2'':5'',2'''-Quaterthiophene]-5,5'''-dicarboxylic acid (9CI) (CA INDEX NAME)



REFERENCE COUNT: 63 THERE ARE 63 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

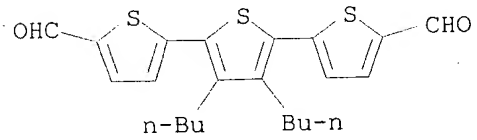
=> d ibib abs hitstr 4

L55 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1996:195129 HCAPLUS
DOCUMENT NUMBER: 124:233307
TITLE: Synthesis and Characterization of A New Conjugated Aromatic Poly(azomethine) Derivative Based on the 3',4'-Dibutyl-.alpha.-Terthiophene Building Block
AUTHOR(S): Wang, Chenggang; Shieh, Seaver; LeGoff, Eugene; Kanatzidis, Mercouri G.
CORPORATE SOURCE: Department of Chemistry, Michigan State University, East Lansing, MI, 48824, USA
SOURCE: Macromolecules (**1996**), 29(9), 3147-56
CODEN: MAMOBX; ISSN: 0024-9297
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A new conjugated arom. poly(azomethine) deriv., poly(3',4'-dibutyl-.alpha.-terthiophene-azomethine-1,4-phenylene-azomethine) (PBTPI), has been prepd. by polycondensation of 2,5''-diformyl-3',4'-dibutyl-2,2':5',2''-terthiophene with 1,4-phenylenediamine under the ethanothermal conditions. The red polycryst. PBTPI was characterized by X-ray diffraction, NMR, FTIR, **UV-visible**-near-IR, photoluminescence, and ESR spectroscopies. PBTPI is partially sol. in THF, giving an orange soln. with an absorption max. (.lambda.max) of 457 nm. In the solid state, PBTPI has an optical band gap of 2.06 eV, which is one of the lowest among poly(azomethines), and is highly sensitive to a strong acid environment. Protonation yields a blue polymer with an optical band gap of 1.61 eV. The polymer is completely sol. in concd. sulfuric acid and nitromethane contg. Lewis acids (e.g., AlCl3), giving blue solns. with .lambda.max of 656 and 638 nm, resp. Iodine-doped PBTPI shows low elec. cond. at the order of 10-7-10-8 S/cm. The properties of PBTPI are compared to other, previously characterized, related polymers.

IT **169565-01-9P**, 2,5''-Diformyl-3',4'-dibutyl-2,2':5',2''-terthiophene
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(monomer; prepn. and optical and elec. properties of **conjugated** arom. poly(azomethine) deriv. based on the 3',4'-dibutyl-.alpha.-terthiophene building block)

RN 169565-01-9 HCAPLUS
CN [2,2':5',2''-Terthiophene]-5,5''-dicarboxaldehyde, 3',4'-dibutyl- (9CI) (CA INDEX NAME)



See L51 query display for explanation of this d que

TRAN 09/871,353

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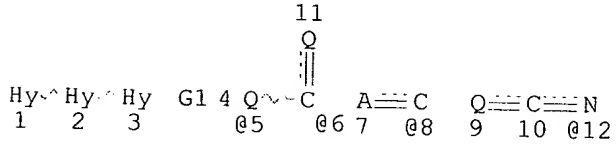
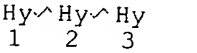
=> d que 156
L1           19 SEA FILE=HCAPLUS ABB=ON  PLU=ON  CIPRIANI F?/AU
L2          135 SEA FILE=HCAPLUS ABB=ON  PLU=ON  GIGLI G?/AU
L3          377 SEA FILE=HCAPLUS ABB=ON  PLU=ON  CINGOLANI R?/AU
L4           48 SEA FILE=HCAPLUS ABB=ON  PLU=ON  FAVARETTO L?/AU
L5           59 SEA FILE=HCAPLUS ABB=ON  PLU=ON  ZAMBIANCHI M?/AU
L6           78 SEA FILE=HCAPLUS ABB=ON  PLU=ON  SOTGIU G?/AU
L7           71 SEA FILE=HCAPLUS ABB=ON  PLU=ON  CITRO G?/AU
L8          132 SEA FILE=HCAPLUS ABB=ON  PLU=ON  BARBARELLA G?/AU
L9          734 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L1 OR L2 OR L3 OR L4 OR L5
                OR L6 OR L7 OR L8)
L10          54 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L9 AND THIOPHENE
L11          30 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L10 AND OLIGOMER?
L12           5 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L11 AND (THIOPHENE OLIGOMER)/T
                I
L13          24 SEA FILE=REGISTRY ABB=ON  PLU=ON  (376393-41-8/BI OR 376393-42-
                9/BI OR 376393-43-0/BI OR 376393-44-1/BI OR 492-97-7/BI OR
                111372-97-5/BI OR 111744-23-1/BI OR 113386-74-6/BI OR 116159-99
                -0/BI OR 118347-89-0/BI OR 127236-47-9/BI OR 127236-48-0/BI OR
                127473-73-8/BI OR 127473-74-9/BI OR 127473-75-0/BI OR 139747-07
                -2/BI OR 139747-08-3/BI OR 14762-74-4/BI OR 201604-95-7/BI OR
                201604-98-0/BI OR 25233-34-5/BI OR 376393-45-2/BI OR 5632-29-1/
                BI OR 67984-20-7/BI)
L14           4 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L12 AND L13
L15           5 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L12 OR L14
L16             STR
```




```
VAR G1=5/6/8/12/NH2/OH/SH/SO3H/SO2
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
GGCAT   IS MCY  UNS  AT   1
GGCAT   IS MCY  UNS  AT   2
GGCAT   IS MCY  UNS  AT   3
DEFAULT ECLEVEL IS LIMITED
ECOUNT  IS E4 C  E1 S  AT   1
ECOUNT  IS E4 C  E1 S  AT   2
ECOUNT  IS E4 C  E1 S  AT   3

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  12

STEREO ATTRIBUTES: NONE
L17       289013 SEA FILE=REGISTRY ABB=ON  PLU=ON  16.145.3/RID
L19              STR
```

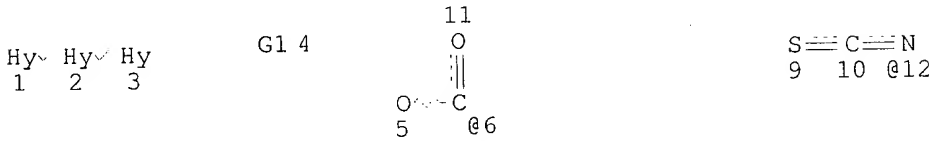


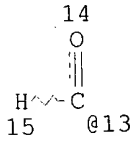

```
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
GGCAT   IS MCY  UNS  AT   1
GGCAT   IS MCY  UNS  AT   2
```

```
GGCAT   IS MCY  UNS  AT   3
DEFAULT ECLEVEL IS LIMITED
ECOUNT  IS E4 C  E1 S  AT   1
ECOUNT  IS E4 C  E1 S  AT   2
ECOUNT  IS E4 C  E1 S  AT   3

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   3

STEREO ATTRIBUTES: NONE
L21         5115 SEA FILE=REGISTRY SUB=L17 SSS FUL L19
L23         2293 SEA FILE=REGISTRY SUB=L21 SSS FUL L16
L26              STR
```






```
VAR G1=OH/SH/NH2/13/6/12
NODE ATTRIBUTES:
CONNECT IS E1  RC AT   5
DEFAULT MLEVEL IS ATOM
GGCAT   IS MCY  UNS  AT   1
GGCAT   IS MCY  UNS  AT   2
GGCAT   IS MCY  UNS  AT   3
DEFAULT ECLEVEL IS LIMITED
ECOUNT  IS E4 C  E1 S  AT   1
ECOUNT  IS E4 C  E1 S  AT   2
ECOUNT  IS E4 C  E1 S  AT   3

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  13

STEREO ATTRIBUTES: NONE
L27         1357 SEA FILE=REGISTRY SUB=L23 SSS FUL L26
L28          476 SEA FILE=REGISTRY ABB=ON  PLU=ON  L27 AND  3 16.145.3/RID
L29          166 SEA FILE=REGISTRY ABB=ON  PLU=ON  L27 AND  4 16.145.3/RID
L30          104 SEA FILE=REGISTRY ABB=ON  PLU=ON  L27 AND  5 16.145.3/RID
L31          746 SEA FILE=REGISTRY ABB=ON  PLU=ON  (L28 OR L29 OR L30)
L32          674 SEA FILE=REGISTRY ABB=ON  PLU=ON  L31 AND NC=1 NOT ("DIAZO" OR
                 F/ELS)
L33        23948 SEA FILE=REGISTRY ABB=ON  PLU=ON  2 16.145.3/RID
L35         2996 SEA FILE=REGISTRY ABB=ON  PLU=ON  L33 AND "BITHIOPHENE"
L38          662 SEA FILE=REGISTRY ABB=ON  PLU=ON  L35 AND ("HYDROXY" OR
                 "HYDROXYL" OR "CARBOXALDEHYDE" OR "FORMYL" OR  "ISOTHIOCYANATO"
                  OR "THIOL" OR "AMINO" OR "CARBOXYLIC") NOT "ESTER"
L39          584 SEA FILE=REGISTRY ABB=ON  PLU=ON  L38 AND NC=1
L40          451 SEA FILE=REGISTRY ABB=ON  PLU=ON  L39 NOT "AZO"
L41          287 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L32
```

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L42	455	SEA FILE=HCAPLUS ABB=ON PLU=ON L40
L43	15	SEA FILE=HCAPLUS ABB=ON PLU=ON L41(L)?CONJUGAT?
L44	14	SEA FILE=HCAPLUS ABB=ON PLU=ON L42(L)?CONJUGAT?
L45	26	SEA FILE=HCAPLUS ABB=ON PLU=ON L43 OR L44
L46	25	SEA FILE=HCAPLUS ABB=ON PLU=ON L45 NOT L15
L47	3042811	SEA FILE=HCAPLUS ABB=ON PLU=ON ANTIBOD? OR FLUORESC?(3A)MARKER OR PROTEIN OR DNA OR NUCLEIC OR OLIGONUC? OR HORMON? OR DRUG OR MEDICINE OR NEUROTRANSMITTER
L48	121828	SEA FILE=HCAPLUS ABB=ON PLU=ON SPECTROFLUORIMETRY OR CYTOMETRY OR FLUORESCENCE(W)MICROSCO? OR GEL ELECTROPHOR?
L49	40	SEA FILE=HCAPLUS ABB=ON PLU=ON (L41 OR L42) AND (L47 OR L48)
L50	8	SEA FILE=HCAPLUS ABB=ON PLU=ON L49 AND ?CONJUGAT?
L51	7	SEA FILE=HCAPLUS ABB=ON PLU=ON L50 NOT L15
L52	20	SEA FILE=HCAPLUS ABB=ON PLU=ON L46 NOT L51
L56	2	SEA FILE=HCAPLUS ABB=ON PLU=ON L52 AND PATENT/DT

2 patents.

Searched by Susan Hanley 305-4053

=> d ibib abs hitstr 1

L56 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2002:172353 HCAPLUS
DOCUMENT NUMBER: 136:238802
TITLE: Second-order nonlinear optical chromophores containing dioxine and/or bithiophene as conjugate bridge and devices incorporating the same
INVENTOR(S): Wang, Chuanguang; Zhang, Cheng; Fetterman, Harold R.; Steier, William; Michael, Joseph
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 16 pp., Cont.-in-part of U. S. Ser. No. 488,422.
CODEN: USXXCO
DOCUMENT TYPE: **Patent**
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 7
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002027220	A1	20020307	US 2001-898625	20010703
US 6067186	A	20000523	US 1998-122806	19980727
US 6361717	B1	20020326	US 2000-488422	20000120
US 6348992	B1	20020219	US 2000-551685	20000418

PRIORITY APPLN. INFO.: US 1998-122806 A2 19980727
US 2000-488422 A2 20000120
US 2000-546930 A2 20000411
US 2000-551685 A2 20000418

OTHER SOURCE(S): MARPAT 136:238802
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

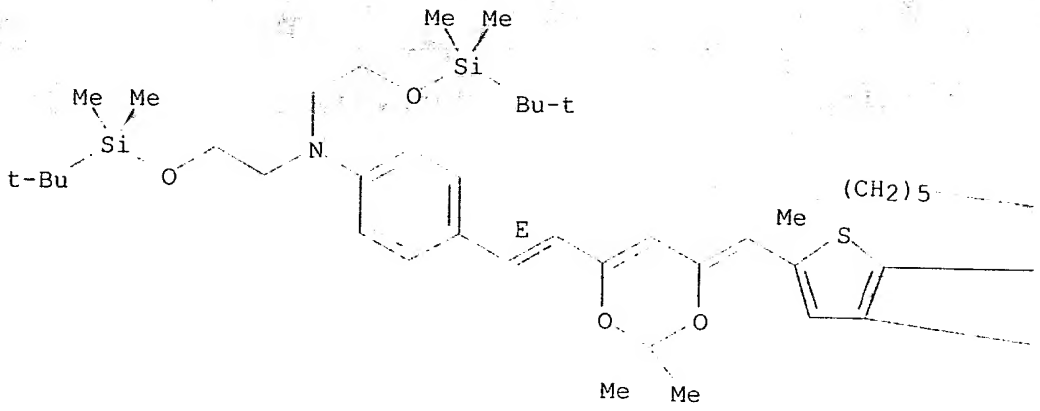
AB Nonlinear optical devices (e.g., electrooptical modulators, phase shifters) comprising an active element formed from a chromophore including an electron donor group, an electron acceptor group, and a bridge structure between the electron donor group and the electron acceptor group are described in which the chromophores is described by the general formula I, the bridge structure is described by the general formula II, or the electron donor group and the bridge structure are described by the general formula III (A = CH2 or O; B = is an electron acceptor; and R = independently selected H, F, or a perhalogenated, halogenated, or nonhalogenated C1-30 aliph. or arom. group functionalized with .gtoreq.0 hydroxy, ether, ester, amino, silyl, and siloxy groups).

IT **392662-52-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(nonlinear optical devices employing second-order nonlinear optical chromophores contg. dioxine and/or bithiophene as **conjugate** bridge)

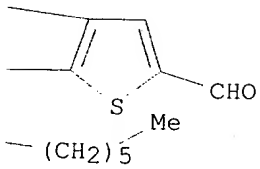
RN 392662-52-1 HCAPLUS
CN [2,2'-Bithiophene]-5-carboxaldehyde, 5'-[[6-[(1E)-2-[4-[bis[2-[[(1,1-dimethylethyl)dimethylsilyl]oxy]ethyl]amino]phenyl]ethenyl]-2,2-dimethyl-4H-1,3-dioxin-4-ylidene]methyl]-3,3'-dihexyl- (9CI) (CA INDEX NAME)

Double bond geometry as described by E or Z.

PAGE 1-A



PAGE 1-B



=> d ibib abs hitstr 2

L56 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2002:90034 HCAPLUS
DOCUMENT NUMBER: 136:136245
TITLE: Hyperpolarizable organic chromophores
INVENTOR(S): Dalton, Larry R.; Jen, Alex Kwan-Yue; Londergan, Timothy; Carlson, William Brenden; Phelan, Gregory; Huang, Diyun; Casmier, Daniel; Ewy, Todd; Buker, Nicholas
PATENT ASSIGNEE(S): University of Washington, USA
SOURCE: PCT Int. Appl., 104 pp.
CODEN: PIXXD2
DOCUMENT TYPE: **Patent**
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002008215	A1	20020131	WO 2001-US23339	20010724
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2002084446	A1	20020704	US 2001-912444	20010724

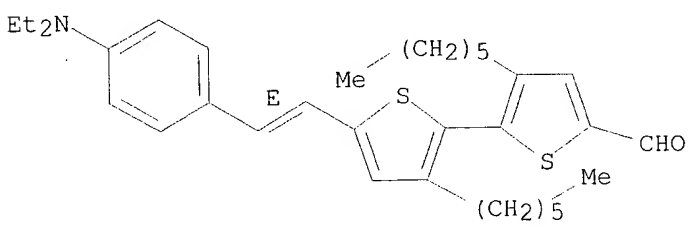
PRIORITY APPLN. INFO.: US 2000-220321P P 20000724
OTHER SOURCE(S): MARPAT 136:136245

AB The present invention provides hyperpolarizable org. chromophores based on heterocyclic compds. The chromophores are nonlinear optically active compds. that include a .pi.-donor conjugated to a .pi.-acceptor through a .pi.-electron conjugated bridge. Macromol. structures including the hyperpolarizable org. chromophores are also provided.

IT **392662-49-6P 392662-52-1P**
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; prodn. of donor-acceptor **conjugated** hyperpolarizable heterocyclic org. chromophores)

RN 392662-49-6 HCAPLUS
CN [2,2'-Bithiophene]-5-carboxaldehyde, 5'-[(1E)-2-[4-(diethylamino)phenyl]ethenyl]-3,3'-dihexyl- (9CI) (CA INDEX NAME)

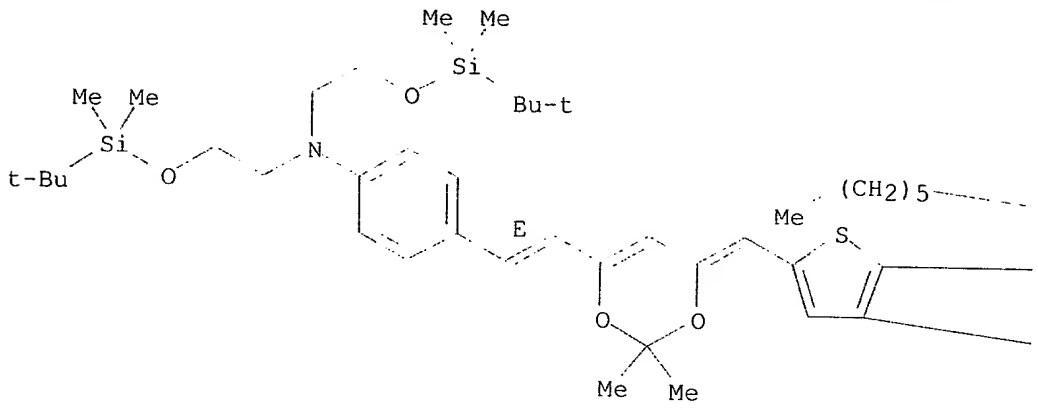
Double bond geometry as shown.



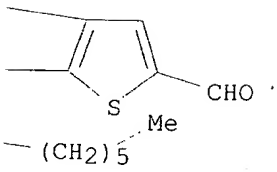
RN 392662-52-1 HCAPLUS
CN [2,2'-Bithiophene]-5-carboxaldehyde, 5'-[[6-[(1E)-2-[4-[bis[2-[[(1,1-dimethylethyl)dimethylsilyl]oxy]ethyl]amino]phenyl]ethenyl]-2,2-dimethyl-4H-1,3-dioxin-4-ylidene]methyl]-3,3'-dihexyl- (9CI) (CA INDEX NAME)

Double bond geometry as described by E or Z.

PAGE 1-A



PAGE 1-B

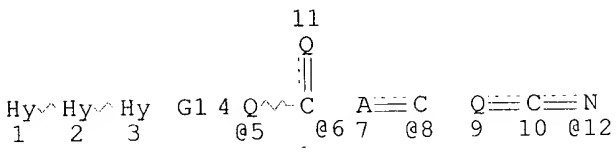


REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

see "d que" for L51 for explanation for this query display

TRAN 09/871,353

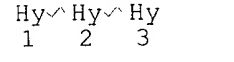
```
=> d que 166 ?
L1            19 SEA FILE=HCAPLUS ABB=ON  PLU=ON  CIPRIANI F?/AU
L2           135 SEA FILE=HCAPLUS ABB=ON  PLU=ON  GIGLI G?/AU
L3           377 SEA FILE=HCAPLUS ABB=ON  PLU=ON  CINGOLANI R?/AU
L4            48 SEA FILE=HCAPLUS ABB=ON  PLU=ON  FAVARETTO L?/AU
L5            59 SEA FILE=HCAPLUS ABB=ON  PLU=ON  ZAMBIANCHI M?/AU
L6            78 SEA FILE=HCAPLUS ABB=ON  PLU=ON  SOTGIU G?/AU
L7            71 SEA FILE=HCAPLUS ABB=ON  PLU=ON  CITRO G?/AU
L8           132 SEA FILE=HCAPLUS ABB=ON  PLU=ON  BARBARELLA G?/AU
L9           734 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L1 OR L2 OR L3 OR L4 OR L5
                 OR L6 OR L7 OR L8)
L10           54 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L9 AND THIOPHENE
L11           30 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L10 AND OLIGOMER?
L12            5 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L11 AND (THIOPHENE OLIGOMER)/T
                 I
L13           24 SEA FILE=REGISTRY ABB=ON  PLU=ON  (376393-41-8/BI OR 376393-42-
                 9/BI OR 376393-43-0/BI OR 376393-44-1/BI OR 492-97-7/BI OR
                 111372-97-5/BI OR 111744-23-1/BI OR 113386-74-6/BI OR 116159-99
                 -0/BI OR 118347-89-0/BI OR 127236-47-9/BI OR 127236-48-0/BI OR
                 127473-73-8/BI OR 127473-74-9/BI OR 127473-75-0/BI OR 139747-07
                 -2/BI OR 139747-08-3/BI OR 14762-74-4/BI OR 201604-95-7/BI OR
                 201604-98-0/BI OR 25233-34-5/BI OR 376393-45-2/BI OR 5632-29-1/
                 BI OR 67984-20-7/BI)
L14            4 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L12 AND L13
L15            5 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L12 OR L14
L16               STR
```




```
VAR G1=5/6/8/12/NH2/OH/SH/SO3H/SO2
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
GGCAT   IS MCY  UNS  AT   1
GGCAT   IS MCY  UNS  AT   2
GGCAT   IS MCY  UNS  AT   3
DEFAULT ECLEVEL IS LIMITED
ECOUNT  IS E4 C  E1 S  AT   1
ECOUNT  IS E4 C  E1 S  AT   2
ECOUNT  IS E4 C  E1 S  AT   3

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  12

STEREO ATTRIBUTES: NONE
L17       289013 SEA FILE=REGISTRY ABB=ON  PLU=ON  16.145.3/RID
L19               STR
```




```
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
GGCAT   IS MCY  UNS  AT   1
GGCAT   IS MCY  UNS  AT   2
```

Searched by Susan Hanley 305-4053

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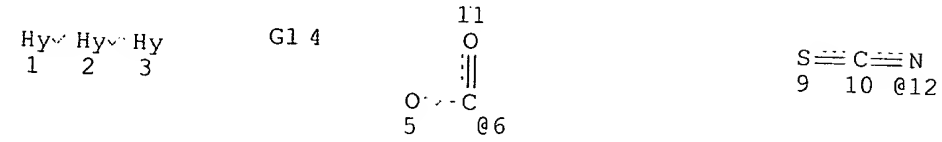
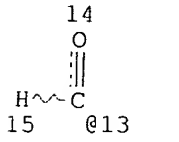
```
GGCAT   IS MCY  UNS  AT   3
DEFAULT ECLEVEL IS LIMITED
ECOUNT  IS E4 C  E1 S  AT   1
ECOUNT  IS E4 C  E1 S  AT   2
ECOUNT  IS E4 C  E1 S  AT   3

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   3

STEREO ATTRIBUTES: NONE
L21         5115 SEA FILE=REGISTRY SUB=L17 SSS FUL L19
L23         2293 SEA FILE=REGISTRY SUB=L21 SSS FUL L16
L26              STR
```






```
VAR G1=OH/SH/NH2/13/6/12
NODE ATTRIBUTES:
CONNECT IS E1  RC AT   5
DEFAULT MLEVEL IS ATOM
GGCAT   IS MCY  UNS  AT   1
GGCAT   IS MCY  UNS  AT   2
GGCAT   IS MCY  UNS  AT   3
DEFAULT ECLEVEL IS LIMITED
ECOUNT  IS E4 C  E1 S  AT   1
ECOUNT  IS E4 C  E1 S  AT   2
ECOUNT  IS E4 C  E1 S  AT   3

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  13

STEREO ATTRIBUTES: NONE
L27         1357 SEA FILE=REGISTRY SUB=L23 SSS FUL L26
L28          476 SEA FILE=REGISTRY ABB=ON  PLU=ON  L27 AND  3 16.145.3/RID
L29          166 SEA FILE=REGISTRY ABB=ON  PLU=ON  L27 AND  4 16.145.3/RID
L30          104 SEA FILE=REGISTRY ABB=ON  PLU=ON  L27 AND  5 16.145.3/RID
L31          746 SEA FILE=REGISTRY ABB=ON  PLU=ON  (L28 OR L29 OR L30)
L32          674 SEA FILE=REGISTRY ABB=ON  PLU=ON  L31 AND NC=1 NOT ("DIAZO" OR
                 F/ELS)
L33        23948 SEA FILE=REGISTRY ABB=ON  PLU=ON  2 16.145.3/RID
L35         2996 SEA FILE=REGISTRY ABB=ON  PLU=ON  L33 AND "BITHIOPHENE"
L38          662 SEA FILE=REGISTRY ABB=ON  PLU=ON  L35 AND ("HYDROXY" OR
                 "HYDROXYL" OR "CARBOXALDEHYDE" OR "FORMYL" OR  "ISOTHIOCYANATO"
                  OR "THIOL" OR "AMINO" OR "CARBOXYLIC") NOT "ESTER"
L39          584 SEA FILE=REGISTRY ABB=ON  PLU=ON  L38 AND NC=1
L40          451 SEA FILE=REGISTRY ABB=ON  PLU=ON  L39 NOT "AZO"
L41          287 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L32
```

Searched by Susan Hanley 305-4053

TRAN 09/871,353

L42	455	SEA FILE=HCAPLUS ABB=ON PLU=ON L40
L43	15	SEA FILE=HCAPLUS ABB=ON PLU=ON L41(L)?CONJUGAT?
L44	14	SEA FILE=HCAPLUS ABB=ON PLU=ON L42(L)?CONJUGAT?
L45	26	SEA FILE=HCAPLUS ABB=ON PLU=ON L43 OR L44
L46	25	SEA FILE=HCAPLUS ABB=ON PLU=ON L45 NOT L15
L47	3042811	SEA FILE=HCAPLUS ABB=ON PLU=ON ANTIBOD? OR FLUORESC?(3A)MARKER OR PROTEIN OR DNA OR NUCLEIC OR OLIGONUC? OR HORMON? OR DRUG OR MEDICINE OR NEUROTRANSMITTER
L48	121828	SEA FILE=HCAPLUS ABB=ON PLU=ON SPECTROFLUORIMETRY OR CYTOMETRY OR FLUORESCENCE(W)MICROSCO? OR GEL ELECTROPHOR?
L49	40	SEA FILE=HCAPLUS ABB=ON PLU=ON (L41 OR L42) AND (L47 OR L48)
L50	8	SEA FILE=HCAPLUS ABB=ON PLU=ON L49 AND ?CONJUGAT?
L51	7	SEA FILE=HCAPLUS ABB=ON PLU=ON L50 NOT L15
L52	20	SEA FILE=HCAPLUS ABB=ON PLU=ON L46 NOT L51
L57	32	SEA FILE=HCAPLUS ABB=ON PLU=ON L49 NOT (L50 OR L52)
L60	20	SEA FILE=HCAPLUS ABB=ON PLU=ON L57 AND THIOPHEN?/OBI
L61	12	SEA FILE=HCAPLUS ABB=ON PLU=ON L57 AND BITHIOPHEN?/OBI
L65	21	SEA FILE=HCAPLUS ABB=ON PLU=ON (L60 OR L61)
L66	2	SEA FILE=HCAPLUS ABB=ON PLU=ON L65 AND (?CONJUGAT? OR LINK? OR COVALENT? OR LIGAND) 2 cites

Searched by Susan Hanley 305-4053

=> d ibib abs hitstr 1

L66 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:384558 HCAPLUS
DOCUMENT NUMBER: 133:28235
TITLE: Preparation of nanoparticles with polymer shells for use in assays
INVENTOR(S): Mirkin, Chad A.; Nguyen, Sonbinh T.
PATENT ASSIGNEE(S): Nanosphere LLC, USA
SOURCE: PCT Int. Appl., 65 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000033079	A1	20000608	WO 1999-US28387	19991130
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1135682	A1	20010926	EP 1999-962951	19991130
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002531830	T2	20020924	JP 2000-585664	19991130

PRIORITY APPLN. INFO.: US 1998-110327P P 19981130
WO 1999-US28387 W 19991130

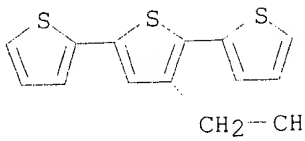
OTHER SOURCE(S): MARPAT 133:28235

AB The invention provides a method of prepg. nanoparticles having at least one polymer shell attached to them, each polymer shell having a selected property or properties. The method comprises attaching initiation monomers to the surfaces of the nanoparticles, contacting the nanoparticles having the initiation monomers attached to them with a transition metal ring-opening metathesis catalyst to activate the initiation monomers, and contacting the nanoparticles with one or more types of propagation monomers of the formula P-L-N under conditions effective so that the monomers are polymd. to form the one or more polymer shells. In the formula P-L-N, N is a cyclic olefin-contg. group, P is a moiety which gives each polymer shell a selected property or properties, and L is a bond or **linker**. The invention also provides polymers formed by polymg. the propagation monomers. The invention further provides the nanoparticles, the initiation monomers, and propagation monomers of formula P-L-N wherein P is a moiety having a property selected from the group consisting of redox activity, optical activity, elec. activity and magnetic activity, and L and N are defined above. The invention also provides binding monomers of formula B-L-N, wherein B is a binding moiety that binds specifically to an analyte, and N and L are defined above. Finally, the invention provides methods and kits for detecting or quantitating an analyte.

IT **273400-09-2**, [2,2':5',2''-Terthiophene]-3'-ethanol
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of nanoparticles with polymer shells for use in assays)

RN 273400-09-2 HCAPLUS

CN [2,2':5',2''-Terthiophene]-3'-ethanol (9CI) (CA INDEX NAME)



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ind

L66 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2002 ACS
IC ICM G01N033-553
ICS B32B005-16
CC 9-1 (Biochemical Methods)
Section cross-reference(s): 35
ST nanoparticle polymer shell assay; binding assay nanoparticle polymer shell; polymn ring opening metathesis polymer shell
IT Analytical apparatus
(for binding assays; prepn. of nanoparticles with polymer shells for use in assays)
IT **Antibodies**
RL: ARG (Analytical reagent use); TEM (Technical or engineered material use); ANST (Analytical study); USES (Uses)
(immobilized; prepn. of nanoparticles with polymer shells for use in assays)
IT Fluorescent substances
(polymer contg.; prepn. of nanoparticles with polymer shells for use in assays)
IT **Oligonucleotides**
RL: ARG (Analytical reagent use); TEM (Technical or engineered material use); ANST (Analytical study); USES (Uses)
(polymer shell-immobilized; prepn. of nanoparticles with polymer shells for use in assays)
IT Cycloalkenes
Nucleic acids
RL: TEM (Technical or engineered material use); USES (Uses)
(polymer shell-immobilized; prepn. of nanoparticles with polymer shells for use in assays)
IT Biosensors
Colorimetry
Fluorometry
Nanoparticles
Nucleic acid hybridization
Redox potential
Test kits
(prepn. of nanoparticles with polymer shells for use in assays)
IT Antigens
Haptens
Nucleic acids
RL: ANT (Analyte); ANST (Analytical study)
(prepn. of nanoparticles with polymer shells for use in assays)
IT Polymers, preparation
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); TEM (Technical or engineered material use); ANST (Analytical study); PREP

(Preparation); USES (Uses)
(prepn. of nanoparticles with polymer shells for use in assays)

IT Polymerization
(ring-opening metathesis; prepn. of nanoparticles with polymer shells for use in assays)

IT 220577-97-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(as initiation monomer; prepn. of nanoparticles with polymer shells for use in assays)

IT 220577-87-7P, exo-5-Norbornen-2-yl ferrocenecarboxylate 220577-89-9P, exo-5-Norbornen-2-yl ferroceneacetate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(as propagation monomer; prepn. of nanoparticles with polymer shells for use in assays)

IT 112-55-0, 1-Dodecanethiol
RL: RCT (Reactant); RACT (Reactant or reagent)
(in prepn. of gold nanoparticles capped with linear alkanethiols; prepn. of nanoparticles with polymer shells for use in assays)

IT 7440-57-5, Gold, uses
RL: TEM (Technical or engineered material use); USES (Uses)
(nanoparticles; prepn. of nanoparticles with polymer shells for use in assays)

IT 172222-30-9
RL: CAT (Catalyst use); USES (Uses)
(prepn. of nanoparticles with polymer shells for use in assays)

IT 220577-91-3DP, gold nanoparticle-immobilized 220577-93-5DP, gold nanoparticle-immobilized 273400-11-6P 273400-13-8P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of nanoparticles with polymer shells for use in assays)

IT 79-37-8, Oxalyl chloride 124-41-4, Sodium methoxide 623-24-5 1271-42-7, Ferrocenecarboxylic acid 1271-86-9, N,N-Dimethylaminomethylferrocene 1287-16-7, Ferroceneacetic acid 2321-07-5, Fluorescein 2890-98-4, exo-5-Norbornen-2-ol 5257-37-4 5713-61-1, (2-Thienyl)magnesiumbromide 6964-21-2, 3-**Thiopheneacetic** acid 7087-68-5, N, N-Diisopropylethylamine 10387-40-3, Potassium thioacetate 13191-37-2 42758-92-9 66605-79-6, 10-Chlorodecyl toluene-4 sulfonate 72287-26-4 89992-70-1 **273400-09-2**, [2,2':5',2''-Terthiophene]-3'-ethanol 273400-12-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of nanoparticles with polymer shells for use in assays)

IT 220577-95-7P 220577-99-1P 273400-05-8P 273400-07-0P 273400-14-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of nanoparticles with polymer shells for use in assays)

IT 220577-91-3P 273400-06-9P 273400-08-1P 273400-10-5P 273400-15-0P 273400-16-1P 273400-17-2P 273932-27-7P 273932-30-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of nanoparticles with polymer shells for use in assays)

IT 50-99-7D, D-Glucose, polymer shell-immobilized, uses 69-79-4D, Maltose, polymer shell-immobilized 99685-96-8D, Fullerene-C60, polymer shell-immobilized
RL: TEM (Technical or engineered material use); USES (Uses)
(prepn. of nanoparticles with polymer shells for use in assays)

IT 16903-35-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(redn. of, in prepn. of gold nanoparticles capped with linear alkanethiols; prepn. of nanoparticles with polymer shells for use in assays)

=> d ibib abs hitstr 2

L66 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1998:709262 HCAPLUS
DOCUMENT NUMBER: 129:326078
TITLE: Use of one-dimensional nuclear magnetic resonance to identify **ligands** to target biomolecules
INVENTOR(S): Fesik, Stephen W.; Hajduk, Philip J.; Olejniczak, Edward T.
PATENT ASSIGNEE(S): Abbott Laboratories, USA
SOURCE: PCT Int. Appl., 28 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

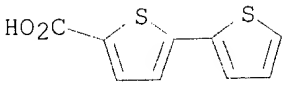
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9848264	A1	19981029	WO 1998-US7907	19980417
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 6043024	A	20000328	US 1997-844124	19970418
ZA 9802919	A	19981012	ZA 1998-2919	19980406
AU 9871380	A1	19981113	AU 1998-71380	19980417
EP 975954	A1	20000202	EP 1998-918461	19980417
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, FI, RO				
BR 9808079	A	20000308	BR 1998-8079	19980417
JP 2002507277	T2	20020305	JP 1998-546228	19980417
NO 9905078	A	19991206	NO 1999-5078	19991018

PRIORITY APPLN. INFO.:
US 1997-844124 A 19970418
WO 1998-US7907 W 19980417

AB The invention provides a process for identifying compds. which bind to a specific target mol. (**protein**, receptor, **nucleic** acid, etc.). The process comprises (a) generating a 1st T2- or diffusion-filtered proton spectrum of 1 or a mixt. of chem. compds.; (b) exposing 1 or a mixt. of chem. compds. to the target mol.; (c) generating a 2nd T2- or diffusion-filtered proton spectrum of 1 or a mixt. of chem. compds. that has been exposed to the target mol. in step (b); and (d) comparing the 1st and 2nd T2- or diffusion-filtered proton spectra to det. differences between the 1st and the 2nd spectra, the differences identifying the presence of .gtoreq.1 compds. that are **ligands** which have bound to the target mol.

IT **2060-55-1**, [2,2'-**Bithiophene**]-5-carboxylic acid
RL: BPR (Biological process); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); BIOL (Biological study); PROC (Process)
(one-dimensional T2- or diffusion-filtered NMR to identify **ligands** to target biomols.)

RN 2060-55-1 HCAPLUS
CN [2,2'-Bithiophene]-5-carboxylic acid (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

TRAN 09/871,353

see the dque for L51 for an explanation of this query display

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=> d que l71
L16                 STR

                      11
                      Q
                      ||
Hy  Hy  Hy  G1 4 Q  -C   A=C   Q=C=N
1   2   3       @5    @6 7   @8   9   10 @12

VAR G1=5/6/8/12/NH2/OH/SH/SO3H/SO2
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
GGCAT   IS MCY  UNS  AT   1
GGCAT   IS MCY  UNS  AT   2
GGCAT   IS MCY  UNS  AT   3
DEFAULT ECLEVEL IS LIMITED
ECOUNT  IS E4 C  E1 S  AT   1
ECOUNT  IS E4 C  E1 S  AT   2
ECOUNT  IS E4 C  E1 S  AT   3

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  12

STEREO ATTRIBUTES: NONE
L17       289013 SEA FILE=REGISTRY ABB=ON  PLU=ON  16.145.3/RID
L19              STR

Hy^Hy^Hy
1  2  3


NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
GGCAT   IS MCY  UNS  AT   1
GGCAT   IS MCY  UNS  AT   2
GGCAT   IS MCY  UNS  AT   3
DEFAULT ECLEVEL IS LIMITED
ECOUNT  IS E4 C  E1 S  AT   1
ECOUNT  IS E4 C  E1 S  AT   2
ECOUNT  IS E4 C  E1 S  AT   3

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   3

STEREO ATTRIBUTES: NONE
L21         5115 SEA FILE=REGISTRY SUB=L17 SSS FUL L19
L23         2293 SEA FILE=REGISTRY SUB=L21 SSS FUL L16
L26              STR
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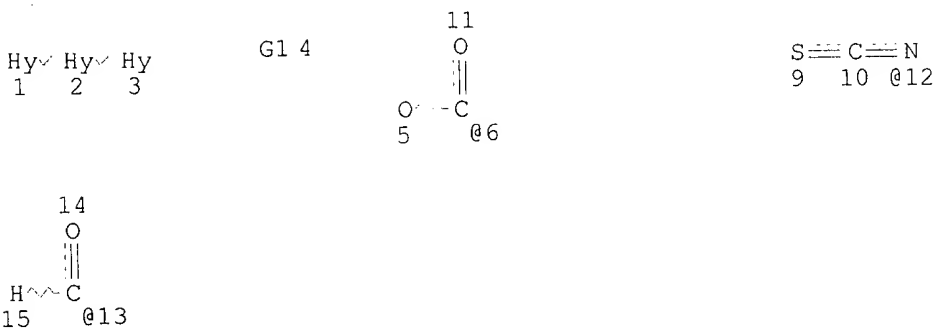
Searched by Susan Hanley 305-4053

TRAN 09/871,353



VAR G1=OH/SH/NH2/13/6/12
NODE ATTRIBUTES:
CONNECT IS E1 RC AT 5
DEFAULT MLEVEL IS ATOM
GGCAT IS MCY UNS AT 1
GGCAT IS MCY UNS AT 2
GGCAT IS MCY UNS AT 3
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS E4 C E1 S AT 1
ECOUNT IS E4 C E1 S AT 2
ECOUNT IS E4 C E1 S AT 3

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE

L27	1357	SEA	FILE=REGISTRY	SUB=L23 SSS FUL L26	
L28	476	SEA	FILE=REGISTRY	ABB=ON	PLU=ON L27 AND 3 16.145.3/RID
L29	166	SEA	FILE=REGISTRY	ABB=ON	PLU=ON L27 AND 4 16.145.3/RID
L30	104	SEA	FILE=REGISTRY	ABB=ON	PLU=ON L27 AND 5 16.145.3/RID
L31	746	SEA	FILE=REGISTRY	ABB=ON	PLU=ON (L28 OR L29 OR L30)
L32	674	SEA	FILE=REGISTRY	ABB=ON	PLU=ON L31 AND NC=1 NOT ("DIAZO" OR F/ELS)
L33	23948	SEA	FILE=REGISTRY	ABB=ON	PLU=ON 2 16.145.3/RID
L35	2996	SEA	FILE=REGISTRY	ABB=ON	PLU=ON L33 AND "BITHIOPHENE"
L38	662	SEA	FILE=REGISTRY	ABB=ON	PLU=ON L35 AND ("HYDROXY" OR "HYDROXYL" OR "CARBOXALDEHYDE" OR "FORMYL" OR "ISOTHIOCYANATO" OR "THIOL" OR "AMINO" OR "CARBOXYLIC") NOT "ESTER"
L39	584	SEA	FILE=REGISTRY	ABB=ON	PLU=ON L38 AND NC=1
L40	451	SEA	FILE=REGISTRY	ABB=ON	PLU=ON L39 NOT "AZO"
L41	287	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L32
L42	455	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L40
L43	15	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L41(L)?CONJUGAT?
L44	14	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L42(L)?CONJUGAT?
L45	26	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L43 OR L44
L67	57	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON (L41 OR L42) AND (VISIBLE(3A)(UV OR ULTRAVIOLET))
L68	52	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L67 NOT (L43 OR L45)
L69	15	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L68 AND (?CONJUGAT? OR LINK? OR COVALENT? OR LIGAND)
L70	15	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L69 NOT PATENT/DT
L71	14	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L70 AND PD<20010530

14 cites

Searched by Susan Hanley 305-4053

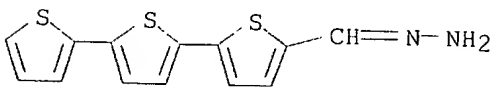
=> d ibib abs hitstr 1-14

L71 ANSWER 1 OF 14 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:755282 HCAPLUS
DOCUMENT NUMBER: 136:207032
TITLE: Spectral characteristics of bisthiophenes and terthiophenes **linked** with heterocyclic unit in solution and polymer matrix
AUTHOR(S): Hrdlovic, Pavol; Krajcovic, Jozef; Vegh, Daniel
CORPORATE SOURCE: Polymer Institute, Slovak Academy of Sciences, Bratislava, 842 36, Slovakia
SOURCE: Journal of Photochemistry and Photobiology, A: Chemistry (**2001**), 144(2-3), 73-82
CODEN: JPPCEJ; ISSN: 1010-6030
PUBLISHER: Elsevier Science S.A.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Spectral characteristics of derivs. of thiophene substituted on hetoroarom. cycle as pyrazine was compared with terthiophene **linked** with cyano- and hydrazo groups. The absorption, fluorescence and its lifetime were measured in soln. (methanol, cyclohexane) and in polymer matrixes (polystyrene, PS; PMMA; and poly(vinyl chloride) (PVC)). Derivs. with two thiophene units substitute on pyrazine exhibit the lowest wavenumber band in the region 26,320-25,600 cm-1 and log .vepsiln. .apprx.4.0, which is not influenced by the medium. Derivs. with benzene and pyridine ring annealed to pyrazine (2,3-bis-(2'-thienyl)quinoxaline (I), 2,3-bis-(2'-thienyl)pyrido[2,3-b]pyrazine (III)) exhibit fluorescence in polar methanol with max. at 22,200 cm-1 and quantum yield of about 0.2 which is blue-shifted in going to non-polar solvent. The max. fluorescence is slightly blue-shifted in polymer matrixes as compared to methanol. Derivs. with annealed thiophene to pyrazine or substituted with two cyano groups (2,3-bis-(2'-thienyl)thieno[3,4-b]pyrazine (II), 2,3-dicyano-5,6-bis(2'-thienyl)pyrazine (IV)) do not yield any emission. Derivs. with terthiophene structural units ([2,2',5',2'']-terthiophene-[2]-thienylacrylonitrile (V) [2,2',5',2'']-terthiophene-5-carbaldehydehydrazone (VI)) exhibit fluorescence with max. around 20,000 cm-1. The lifetime of fluorescence of all thiophene was 1 ns or shorter. The polymer matrixes increase the intensity of fluorescence to some extent and prolong the lifetime of thiophene derivs. Deriv. VI exhibits some tendency to an aggregation at higher concn. above 0.01 mol kg-1 in polymer matrixes.

IT **188123-63-9P**, [2,2',5',2'']-Terthiophene-5-carbaldehydehydrazone
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(optical absorption and emission and lifetime of emission of bis-thiophenes and ter-thiophenes **linked** by heterocyclic unit studied in solns. and in polymer matrixes)

RN 188123-63-9 HCAPLUS
CN [2,2':5',2''-Terthiophene]-5-carboxaldehyde, hydrazone (9CI) (CA INDEX NAME)



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

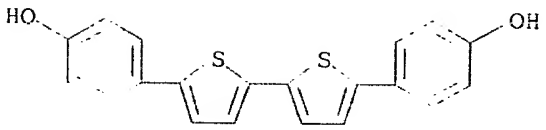
L71 ANSWER 2 OF 14 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:313940 HCAPLUS
DOCUMENT NUMBER: 135:161594
TITLE: Electronic and magnetic metal-metal interactions in dinuclear oxomolybdenum(V) complexes across bis-phenolate bridging **ligands** with different spacers between the phenolate termini: **ligand**-centered vs. metal-centered redox activity
AUTHOR(S): Bayly, Simon R.; Humphrey, Elizabeth R.; de Chair, Helena; Paredes, Cecilia G.; Bell, Zoe R.; Jeffery, John C.; McCleverty, Jon A.; Ward, Michael D.; Totti, Federico; Gatteschi, Dante; Courric, Stephane; Steele, Barry R.; Screttas, Constantinos G.
CORPORATE SOURCE: School of Chemistry, University of Bristol, Bristol, BS8 1TS, UK
SOURCE: Journal of the Chemical Society, Dalton Transactions (**2001**), (9), 1401-1414
CODEN: JCSDAA; ISSN: 1472-7773
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Dinuclear complexes were prepd. in which two {MoV(TpMe,Me)(O)Cl} fragments (abbreviated as Mo; TpMe,Me = tris(3,5-dimethylpyrazol-1-yl)hydroborate) are attached to either end of a bis-p-phenolate bridging **ligand** [(4,4'-OC6H4)-X-(4,4'-C6H4O)]2-. The complexes are Mo2(C:C) (X = CH:CH), Mo2(C:C)2 (X = CH:CH-CH:CH), Mo2(C:C)3 (X = CH:CH-CH:CH-CH:CH), Mo2(th) (X = 2,5-thiophenediyl), Mo2(th)2 (X = 2,5:2',5'-bithiophenediyl), Mo2(th)3 (X = 2,5:2',5':2'',5''-terthiophenediyl), Mo2(C.tplbond.C) (X = C.tplbond.C), Mo2(N:N) (X = N:N), Mo2(CO) [X = C(O)] and Mo2(C2.PHI.C2) [X = CH:CH(1,4-C6H4)CH:CH]. Electrochem., **UV/visible**/NIR spectroelectrochem. and magnetic measurements were carried out to see how effectively the different spacer groups X mediate electronic and magnetic interactions between the two redox-active, paramagnetic, Mo centers. The electronic interactions were detd. from the redox sepn. between the two successive 1-electron oxidns. which are formally Mo(VI)-Mo(V) couples; thienyl units in the bridging **ligand** are much more effective at maintaining electronic communication over long distances than p-phenylene or ethenyl spacers of comparable lengths. The azo (N:N) **linkage** afforded a much weaker electronic interaction than the ethenyl or ethynyl spacers. **UV/visible**/NIR spectroelectrochem. studies showed that whereas the 1st oxidn. is metal-centered to give Mo(VI)-Mo(V) species with characteristic intense phenolate Mo(VI) LMCT transitions in the near-IR region, the spectra of the doubly oxidized complexes are characteristic of quinones: thus, the sequence of species formed on oxidn. is [Mo(V)(.mu.-diolate)Mo(V)]0 .fwdarw. [Mo(V)(.mu.-diolate)Mo(VI)]+ .fwdarw. [Mo(V)(.mu.-quinone)Mo(V)]2+, with an internal charge redistribution assocd. with the 2nd oxidn. Semi-empirical ZINDO calcns. provide some support for this. Magnetic susceptibility measurements on Mo2(C:C), Mo2(th), Mo2(N:N) and Mo2(C.tplbond.C) show that all are weakly antiferromagnetically coupled, as expected from a spin-polarization picture, with the order of strength of the magnetic interaction being the reverse of the order for electronic coupling, such that Mo2(th) affords the strongest electronic interaction but the weakest magnetic interaction.

IT **185413-64-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant for prepn. of oxomolybdenum(V) tris(dimethylpyrazolyl)hydrobo rato chloro dinuclear complex bridged by bis-phenolato **ligand**)

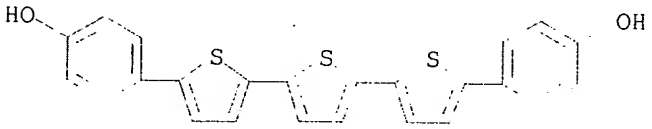
RN 185413-64-3 HCAPLUS

CN Phenol, 4,4'-[2,2'-bithiophene]-5,5'-diylbis- (9CI) (CA INDEX NAME)



IT **352462-92-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(reactant for prepn. of oxomolybdenum(V) tris(dimethylpyrazolyl)hydrobo rato chloro dinuclear complex bridged by bis-phenolato **ligand**)

RN 352462-92-1 HCAPLUS
CN Phenol, 4,4'-[2,2':5',2''-terthiophene]-5,5''-diylbis- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 96 THERE ARE 96 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

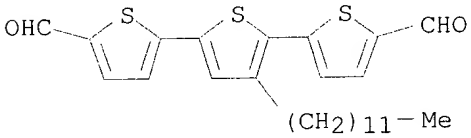
L71 ANSWER 3 OF 14 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:367325 HCAPLUS
DOCUMENT NUMBER: 133:73758
TITLE: Photoinduced Energy and Electron Transfer in Fullerene-Oligothiophene-Fullerene Triads
AUTHOR(S): Van Hal, Paul A.; Knol, Joop; Langeveld-Voss, Bea M. W.; Meskers, Stefan C. J.; Hummelen, J. C.; Janssen, Rene A. J.
CORPORATE SOURCE: Laboratory of Macromolecular and Organic Chemistry, Eindhoven University of Technology, Eindhoven, 5600 MB, Neth.
SOURCE: Journal of Physical Chemistry A (2000), 104(25), 5974-5988
CODEN: JPCAFH; ISSN: 1089-5639
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A series of fullerene-oligothiophene-fullerene (C60-nT-C60) triads with n = 3, 6, or 9 thiophene units has been synthesized, and their photophys. properties have been studied using photoinduced absorption and fluorescence spectroscopy in soln. and in the solid state as thin films. The results are compared to those of mixts. of oligothiophenes (nT) with N-methylfulleropyrrolidine (MP-C60). Photoexcitation of the triads in the film results in an electron-transfer reaction for n = 6 and 9, but not for n = 3. The lifetime of the charge-sepd. state in the film is on the order of milliseconds. Photoexcitation of the oligothiophene moiety of the C60-nT-C60 triads, dissolved in an apolar solvent, results in a singlet energy-transfer reaction to the fullerene moiety with rates varying between 1012 and 1013 s-1. In more polar solvents, an intramol.

photoinduced charge sepn. occurs for n = 6 and 9 and, to some extent, for n = 3. The quenching of the MP-C60(S1) fluorescence provides a lower limit to the rate of the intramol. photoinduced electron transfer of 1011 s-1 in the C60-nT-C60 triads with n = 6 or 9 in polar solvents, assuming that charge sepn. occurs after singlet energy transfer from nT(S1) to MP-C60(S1). A direct mechanism, i.e., charge sepn. from nT(S1), cannot be excluded exptl. but must occur in the femtosecond time domain to compete effectively with energy transfer. The lifetime of the intramolecularly charge-sepd. state in the C60-nT-C60 triads is significantly reduced compared to the lifetime of the radical ions in the films, and hence, the latter results from charge migration to different mol. sites. Similar energy- and electron-transfer reactions occur intermolecularly in soln. from the nT and MP-C60 triplet states. The preferences for intra- and intermol. energy- and electron-transfer reactions, as a function of **conjugation** length and solvent permittivity, are in full agreement with predictions that can be made using the Weller equation for the change in free energy upon charge sepn.

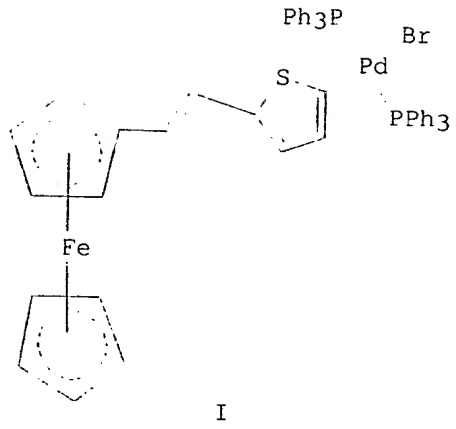
IT **252684-40-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(Prato reaction in regioisomer mixt.; photoinduced energy and electron transfer in fullerene-oligothiophene-fullerene triads)

RN 252684-40-5 HCAPLUS
CN [2,2':5',2''-Terthiophene]-5,5''-dicarboxaldehyde, 3'-dodecyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 103 THERE ARE 103 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L71 ANSWER 4 OF 14 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1999:712697 HCAPLUS
DOCUMENT NUMBER: 132:64385
TITLE: Ferrocene End-Capped Palladium(II) and Platinum(II) Complexes with Thiophene Spacers
AUTHOR(S): Thomas, K. R. Justin; Lin, Jiann T.; Lin, Kuan-Jiuh
CORPORATE SOURCE: Institute of Chemistry, Academia Sinica, Taipei, 115, Taiwan
SOURCE: Organometallics (**1999**), 18(25), 5285-5291
CODEN: ORGND7; ISSN: 0276-7333
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



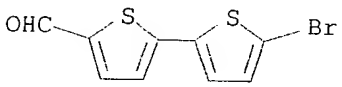
I

AB Heterobimetallics contg. ferrocene and Pd(II) or Pt(II), e.g., I, were synthesized by oxidative addn. of ferrocene-substituted halothiophenes with zerovalent Pd or Pt precursors. The stable solids were thoroughly characterized by elemental anal., NMR, **UV-visible** spectroscopy, and cyclic voltammetry. The rich redox chem. of the complexes depends on the **conjugation** length that separates the two metal sites. The crystal structure of a Pt .sigma.-thienyl complex I was detd.

IT **110046-60-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(Wittig reaction with (ferrocenylmethyl)triphenylphosphonium bromide)

RN 110046-60-1 HCAPLUS

CN [2,2'-Bithiophene]-5-carboxaldehyde, 5'-bromo- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L71 ANSWER 5 OF 14 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1999:305626 HCAPLUS

DOCUMENT NUMBER: 131:58548

TITLE: Intramolecular energy transfer of [60]fullerene-**linked** oligothiophenes

AUTHOR(S): Yamashiro, Takashi; Aso, Yoshio; Otsubo, Tetsuo; Tang, Heqing; Harima, Yutaka; Yamashita, Kazuo

CORPORATE SOURCE: Faculty of Engineering, Hiroshima University, Higashi-Hiroshima, 739-8527, Japan

SOURCE: Chemistry Letters (**1999**), (5), 443-444
CODEN: CMLTAG; ISSN: 0366-7022

PUBLISHER: Chemical Society of Japan

DOCUMENT TYPE: Journal

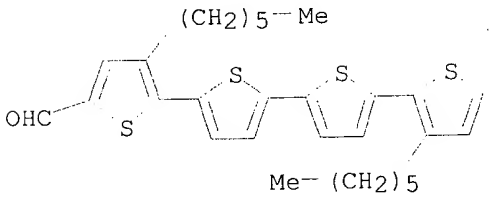
LANGUAGE: English

AB [60]Fullerene-**linked** quarter-, octi-, and duodecithiophenes have been synthesized, and their emission spectra demonstrate efficient intramol. energy transfer from the thiophene moiety to the fullerene, whose rate const. largely depends on the chain length of the

oligothiophene moiety.

IT **228414-99-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of [60]fullerene-**linked** oligothiophenes and chain-length dependence of their intramol. energy transfer assessed from fluorescence quenching measurements)

RN 228414-99-1 HCAPLUS
CN [2,2':5',2'':5'',2'''-Quaterthiophene]-5-carboxaldehyde, 3,3'''-dihexyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L71 ANSWER 6 OF 14 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1998:786650 HCAPLUS
DOCUMENT NUMBER: 130:139711
TITLE: A Novel Series of p-n Diblock Light-Emitting Copolymers Based on Oligothiophenes and 1,4-Bis(oxadiazolyl)-2,5-dialkyloxybenzene
AUTHOR(S): Huang, Wei; Meng, Hong; Yu, Wang-Lin; Pei, Jian; Chen, Zhi-Kuan; Lai, Yee-Hing
CORPORATE SOURCE: Institute of Materials Research and Engineering and Department of Chemistry, National University of Singapore, Singapore, 119260, Singapore
SOURCE: Macromolecules (**1999**), 32(1), 118-126
CODEN: MAMOBX; ISSN: 0024-9297
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A new series of p-n diblock **conjugated** copolymers consisting of alternate 1,4-bis(oxadiazolyl)-2,5-dialkyloxybenzene and oligothiophenes with one to three thiophene rings (P1-P3) have been synthesized. The polymers have well-defined structures and exhibit good thermal stability with the onset decompn. temps. in nitrogen at around 300 .degree.C. The glass transition temp. (Tg) of the polymers decreases with increasing the length of oligothiophene blocks. Both the absorption spectra and photoluminescence spectra shift to longer wavelength with increase in the length of oligothiophene blocks. The emissive color of the polymers could be tuned from blue to green to orange just by increasing the no. of thiophene rings in the oligothiophene blocks from one to three. No obvious change in redn. potential is found for the polymers with variation in the length of oligothiophene blocks. The redn. potential E1/2 of the polymers is measured by cyclic voltammetry to be around -1.7 V vs SCE, comparable to those of poly(cyanoterephthalyidene) (CN-PPV) and other good electron-transporting materials. The oxidn. potential of the polymers can be reduced remarkably by increasing the length of oligothiophene blocks. The oxidn. potential E1/2 of P3 is measured to be 1.25 V with the onset potential at 1.0 V vs SCE. These values are comparable to those of some hole-injection favorable electroluminescent polymers. The results prove

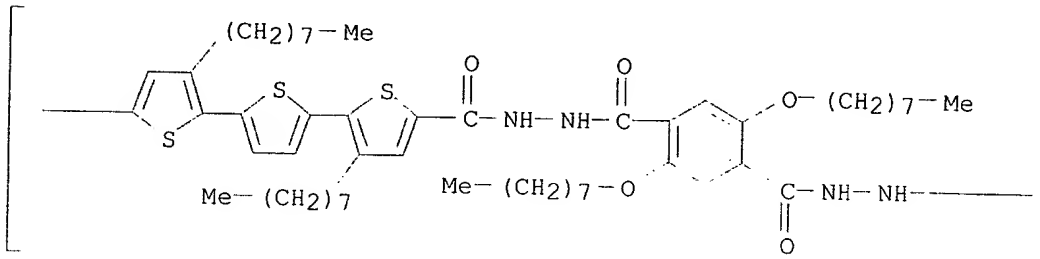
that the p-n diblock structure may be a promising mol. design for synthetically tuning the HOMO and LUMO of **conjugated** polymers.

IT **215324-18-8P**
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and physicochem. properties of series of light-emitting copolymers based on oligothiophenes and 1,4-bis(oxadiazolyl)-2,5-dialkyloxybenzene)

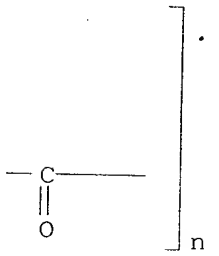
RN 215324-18-8 HCAPLUS

CN Poly[(3,3''-dioctyl[2,2':5',2''-terthiophene]-5,5''-diyl)carbonylhydrazocarbonyl[2,5-bis(octyloxy)-1,4-phenylene]carbonylhydrazocarbonyl] (9CI) (CA INDEX NAME)

PAGE 1-A



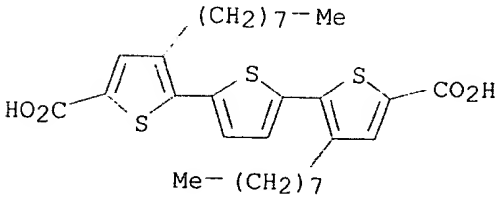
PAGE 1-B



IT **216772-47-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(reactant in monomer prepn.; prepn. and physicochem. properties of series of light-emitting copolymers based on oligothiophenes and 1,4-bis(oxadiazolyl)-2,5-dialkyloxybenzene)

RN 216772-47-3 HCAPLUS

CN [2,2':5',2''-Terthiophene]-5,5''-dicarboxylic acid, 3,3''-dioctyl- (9CI) (CA INDEX NAME)



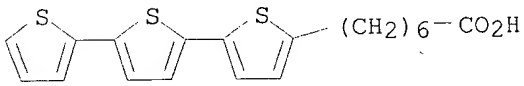
REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L71 ANSWER 7 OF 14 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1998:786594 HCAPLUS
DOCUMENT NUMBER: 130:102060
TITLE: Adsorption of Carboxyl-Terminated Dithiophene and Terthiophene Molecules on ITO Electrodes and Their Electrochemical Coupling to Polymer Layers. The Influence of Molecular Geometry
AUTHOR(S): Berlin, Anna; Zotti, Gianni; Schiavon, Gilberto; Zecchin, Sandro
CORPORATE SOURCE: Centro CNR di Sintesi e Stereochimica di Speciali Sistemi Organici, Milan, 20133, Italy
SOURCE: Journal of the American Chemical Society (**1998**), 120(51), 13453-13460
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Carboxypentyl and carboxyhexyl bithiophenes and terthiophenes, in which the oligothiophene tail is either perpendicularly or linearly **linked** to the tethering carboxyalkyl chain, were adsorbed on ITO electrodes. The obtained stable monolayers are anodically oxidized in acetonitrile to produce polymer layers (storing a reversible charge of 15 .mu.C cm-2) in the case of perpendicular adsorbates whereas linear bithiophene and terthiophene are able to couple only with oligothiophenes in soln. Electrochem. and **UV-visible** spectroscopic anal. indicate that the polymer layers are in fact constituted by thiophene hexamers. The adsorbed linear terthiophene may be coupled with the terthiophene itself in soln. to produce a 1-end surface-grafted sexithiophene monolayer (reversible charge 40 .mu.C cm-2), whereas a two-end surface-grafted sexithiophene with the same coverage is produced by adsorption of the .alpha.-coupled terthiophene. The 1-end and two-end grafted sexithiophene monolayers display different electrochem. and spectral patterns. Chronoamperometry and cyclic voltammetry show that the adsorbed linear bithiophene may be oxidatively coupled with 2,2'-bithiophene in soln. to produce surface-anchored polythiophene chains.

IT **219535-15-6P**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(prepn. and adsorption of carboxyl-terminated dithiophene and terthiophene mols. on ITO electrodes and electrochem. coupling to polymer layers: influence of mol. geometry)

RN 219535-15-6 HCAPLUS
CN [2,2':5',2''-Terthiophene]-5-heptanoic acid (9CI) (CA INDEX NAME)



REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

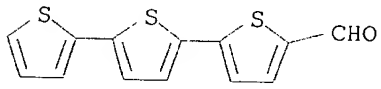
L71 ANSWER 8 OF 14 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1998:752380 HCAPLUS
DOCUMENT NUMBER: 130:167979
TITLE: Investigation of exciton coupling in oligothiophenes by circular dichroism spectroscopy
AUTHOR(S): Langeveld-Voss, Bea M. W.; Beljonne, David; Shuai, Zhigang; Janssen, Rene A. J.; Meskers, Stefan C. J.; Meijer, E. W.; Bredas, Jean-Luc
CORPORATE SOURCE: Lab. Macromolecular Organic Chemistry, Eindhoven Univ. Technology, Eindhoven, 5600 MB, Neth.
SOURCE: Advanced Materials (Weinheim, Germany) (1998), 10(16), 1343-1348
CODEN: ADVMEW; ISSN: 0935-9648
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English

AB To study the effect of exciton coupling on thiophene chromophores, the model compds. N,N'-bis([2,2';5',2'']terthiophen-5''-ylmethylene)cyclohexane-(1S,2S)-diamine (I) and (1R-phenylethyl)-[2,2';5',2'']terthiophen-5''-ylmethylene amine were prepd. and characterized by UV, CD, and fluorescence spectroscopy which were also theor. simulated. The bisignate CD spectrum of I resulted from a right-handed chiral orientation of the 2 terthienyl units with respect to each other. The exciton coupling in I was .apprxeq.0.15-0.2 eV. These observations were consistent with the explanation that the bisignate CD spectra in .pi.-**conjugated** polymers with optically active pendant side chains were caused by a chiral superstructure of predominantly planar chains. Since the CD spectra of I and those of optically active **conjugated** polymers looked alike, it was assumed that the exciton coupling should be of the same order of magnitude.

IT **7342-41-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of oligothiophenes and their exciton coupling studied by CD)

RN 7342-41-8 HCAPLUS
CN [2,2':5',2''-Terthiophene]-5-carboxaldehyde (7CI, 8CI, 9CI) (CA INDEX NAME)



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L71 ANSWER 9 OF 14 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1998:186798 HCAPLUS
DOCUMENT NUMBER: 128:167880
TITLE: Alternating **Conjugated** and **Nonconjugated** Polymer. 1. Crystal Structures and Polymorphism of Poly(hexamethylene 2,2,-bithiophene-5,5,-dicarboxylate), P6BT
AUTHOR(S): Wang, Shanger; Brisse, Francois
CORPORATE SOURCE: Departement de Chimie, Universite de Montreal, Montreal, QC, H3C 3J7, Can.
SOURCE: Macromolecules (1998), 31(7), 2265-2277
CODEN: MAMOBX; ISSN: 0024-9297
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal

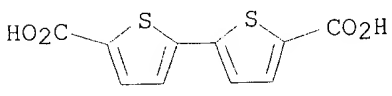
LANGUAGE: English

AB X-ray fiber diffraction and DSC investigations of the title polymer, P6BT, reveal the existence of three polymorphs. Both .alpha.- and .beta.-forms belong to the monoclinic system, while in the .gamma.-form, the chains are packed in a triclinic unit cell. In all three forms the bithiophenedicarboxylate group is confined in a .pi.-**conjugated** plane; however, with different orientations of the carbonyl group relative to the sulfur atom (in .alpha.- and .beta.-froms, S-C-C:O is in the cis conformation, while in the .gamma.-form, S-C-C:O is trans). The methylenic sequence in the .beta.- and .gamma.-forms is in the all-trans conformation with only slight deviations from planarity. With a torsion (.tau.3) around the C-O bond between the arom. plane and aliph. segment, the polymer chain changes its overall shape from ribbonlike in the .alpha.-form (.tau.3 .apprxeq. 180.degree.) to a sine-curve shape in the .beta.-form (.tau.3 = 173.degree.) and finally to a zigzag in the .gamma.-form (.tau.3 = 103.degree.). The .alpha.-form is paracryst., with random displacements of the chains along the fiber axis. The four chains in the unit cell of the .beta.-form are found in two pairs displaced by 5.63 .ANG. from each other, in the c-axis direction. Within the pair, the chains adopt an antiparallel disposition. The arom. planes are arranged nearly parallel to the ac plane in a "side-by-side" pattern in the a-direction. Chains in the .gamma.-form pack in successive layers, where the bithiophene dicarboxylic planes aggregate in a "face-to-face" fashion, forming well-organized .pi.-stacks favorable for the interchain charge transfer of the alternating **conjugated** and **nonconjugated** polymer. The interplanar distance between neighboring bithiophene planes is 3.56 .ANG.. The chain conformation and crystal packing in the .gamma.-form resemble those obsd. in the model compd., di-n-hexyl 2,2'-bithiophene-5,5'-dicarboxylate (6BT6). A monotropic mesophase with unique chain arrangements was found to occur during heating. The transformation temps. are as follows: .alpha.- to .beta.-form, 130-150 .degree.C; .beta.- to .gamma.-form, 161 .degree.C; .gamma.-form to mesophase, 172 .degree.C; and mesophase to isotropic liq., around 185 .degree.C. The strong .pi.-.pi. interaction between arom. planes is believed to be the main driving force of the phase transformations. Due to this solid-state ordering process, the bathochromic shift in the **UV-visible** region was obsd. Some abnormal phenomena such as preferred tilt of crystal in the .gamma.-form are described. The relationship between these structures and those of the biphenyl analog, poly(hexamethylene 4,4'-biphenyldicarboxylate) are discussed.

IT **3515-34-2P**, 2,2'-Bithiophene-5,5'-dicarboxylic acid
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(crystal structures and polymorphism of poly(hexamethylene 2,2,-bithiophene-5,5,-dicarboxylate))

RN 3515-34-2 HCAPLUS

CN [2,2'-Bithiophene]-5,5'-dicarboxylic acid (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



L71 ANSWER 10 OF 14 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1997:324841 HCAPLUS
DOCUMENT NUMBER: 127:34576
TITLE: Low Optical Bandgap Polythiophenes by an Alternating

Donor/Acceptor Repeat Unit Strategy

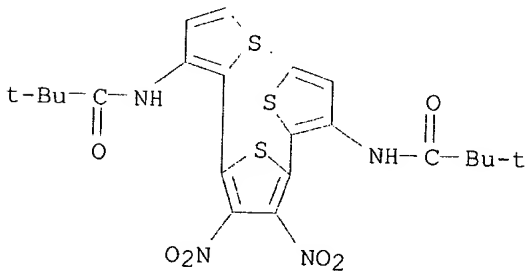
AUTHOR(S): Zhang, Qing; Tour, James M.
CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of South Carolina, Columbia, SC, 29208, USA

SOURCE: Journal of the American Chemical Society (1997), 119(21), 5065-5066
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

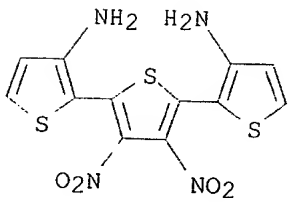
AB This paper describes a method to increase delocalization between consecutive repeat units in **conjugated** polymers by constructing alternating step growth [AB] polymers where the A-units are electron rich and the B-units are electron deficient. The low optical bandgap polymers based on polythiophenes are prepd. by a modified Stille polymn. using a Pd(0) and CuI pre-catalyst system in which aryl dibromides couple with aryl distannanes. The donor units are 3,4-diaminothiophene or an N,N'-bis(tert-butoxycarbonyl)-3,4-diaminothiophene, and the acceptor units are 3,4-dinitrothiophene or a 3,4-n-butylimidothiophene. The optical spectra show .lambda.max values ranging from 526-662 nm, consistent with a decrease in the bandgap. The nitro-contg. polymer is only sol. in polar solvents such as methanol, DMSO, and water, suggesting significant zwitterionic character. Several model trimers were prepd. which have significantly shorter wavelength optical absorptions, thus confirming the need for the extended polymeric systems.

IT **190723-21-8 190723-23-0**
RL: PRP (Properties)
(model compd.; prepn. of low optical bandgap polythiophenes by an alternating donor-acceptor repeat unit strategy)

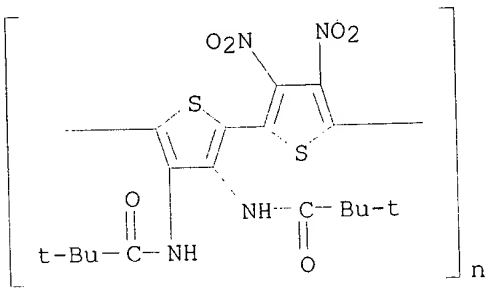
RN 190723-21-8 HCAPLUS
CN Propanamide, N,N'-(3',4'-dinitro[2,2':5',2''-terthiophene]-3,3''-diyl)bis[2,2'-dimethyl- (9CI) (CA INDEX NAME)



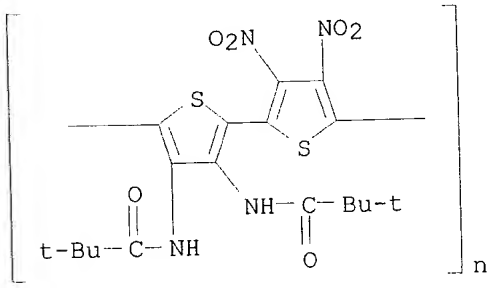
RN 190723-23-0 HCAPLUS
CN [2,2':5',2''-Terthiophene]-3,3''-diamine, 3',4'-dinitro- (9CI) (CA INDEX NAME)



IT **190723-08-1P**
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of low optical bandgap polythiophenes by an alternating donor-acceptor repeat unit strategy)
RN 190723-08-1 HCAPLUS
CN Poly[3,4-bis[(2,2-dimethyl-1-oxopropyl)amino]-3',4'-dinitro[2,2'-bithiophene]-5,5'-diyl] (9CI) (CA INDEX NAME)



IT **190723-08-1DP**, deprotected
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of low optical bandgap polythiophenes by an alternating donor-acceptor repeat unit strategy)
RN 190723-08-1 HCAPLUS
CN Poly[3,4-bis[(2,2-dimethyl-1-oxopropyl)amino]-3',4'-dinitro[2,2'-bithiophene]-5,5'-diyl] (9CI) (CA INDEX NAME)



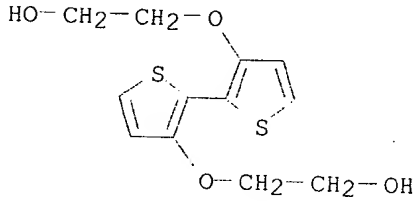
L71 ANSWER 11 OF 14 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1995:797754 HCAPLUS
DOCUMENT NUMBER: 123:352978
TITLE: Ionoresistivity as a highly sensitive sensory probe: investigations of polythiophenes functionalized with calix[4]arene-based ion receptors
AUTHOR(S): Marsella, Michael J.; Newland, Robert J.; Carroll, Patrick J.; Swager, Timothy M.
CORPORATE SOURCE: Department of Chemistry, University of Pennsylvania, Philadelphia, PA, 19104-6323, USA
SOURCE: Journal of the American Chemical Society (**1995**), 117(39), 9842-8
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The authors report the synthesis, optical, and electrochem. properties of a calix[4]arene-substituted polythiophene which demonstrates ion-selective voltammetric, chromic, fluorescent, and resistive responses. The ionochromic response of this polythiophene on exposure to Na+ shows an increased effective **conjugation** length of the polymer backbone. Despite this, Na+ induces a large pos. shift in the potential at which the polymer is oxidized (greater than +100 mV) commensurate with a large decrease in cond. (>99%). Although the calix[4]arene-substituted polythiophene exhibits no changes in the **UV-visible** spectrum and only minimal changes in the voltammetric responses on exposure to Li+ or K+, there are large decreases in relative conductivities (69 and 47%, resp.). Thus, although the sensory properties of this polymer are expressed via several measurable entities, the ionoresistive response is clearly the most sensitive. This sensitivity originates from the cooperative nature of carrier transport in a conducting polymers (CP) and is thus inherent in chemoresistive CPs.

IT **171085-61-3P**, 3,3'-Bis(2-hydroxyethoxy)-2,2'-bithiophene
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and NMR spectra of polythiophene receptors)

RN 171085-61-3 HCAPLUS

CN Ethanol, 2,2'-[[2,2'-bithiophene]-3,3'-diylbis(oxy)]bis- (9CI) (CA INDEX NAME)



L71 ANSWER 12 OF 14 HCAPLUS COPYRIGHT 2002 ACS

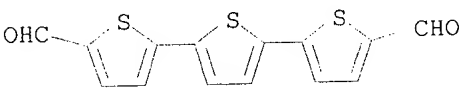
ACCESSION NUMBER: 1995:699277 HCAPLUS
DOCUMENT NUMBER: 123:83040
TITLE: Synthesis and Energy Transfer Properties of Terminally Substituted Oligothiophenes
AUTHOR(S): Wuerthner, Frank; Vollmer, Martin Siegfried; Effenberger, Franz; Emele, Peter; Meyer, Dirk Uwe; Port, Helmut; Wolf, Hans Christoph
CORPORATE SOURCE: Institut fuer Organische Chemie, Universitaet Stuttgart, Stuttgart, D-70569, Germany
SOURCE: Journal of the American Chemical Society (**1995**), 117(31), 8090-9
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A series of **conjugated** anthryl-oligothienyl-porphyrins in which the oligothiophene is terminally **linked** to the 5-position of a porphyrin and to the 9-position of anthracene has been synthesized, and photoexcited-state properties have been studied by steady-state fluorescence spectra, fluorescence excitation spectra and picosecond time-resolved fluorescence measurements. Due to the spectral position of the anthracene and the porphyrin absorption bands a selective excitation of both end groups is possible, which is demonstrated by the **UV-visible** absorption spectra. Selective excitation of the anthryl end group leads to a quant. intramol. energy transfer to the porphyrin end

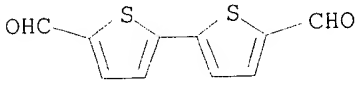
group in the subpicosecond time scale. The mechanism is discussed in terms of existing theories (Forster/Dexter, superexchange, and intramol. relaxation).

IT **13130-50-2P 32364-72-0P**, [2,2'-Bithiophene]-5,5'-dicarboxaldehyde
RL: BYP (Byproduct); PREP (Preparation)
(synthesis and energy transfer properties of anthryl-oligothienyl-porphyrins)

RN 13130-50-2 HCAPLUS
CN [2,2':5',2''-Terthiophene]-5,5''-dicarboxaldehyde (8CI, 9CI) (CA INDEX NAME)

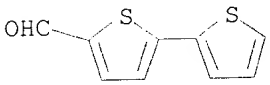


RN 32364-72-0 HCAPLUS
CN [2,2'-Bithiophene]-5,5'-dicarboxaldehyde (7CI, 8CI, 9CI) (CA INDEX NAME)

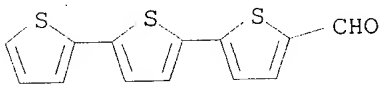


IT **3779-27-9**, 5-Formyl-2,2'-bithiophene **7342-41-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis and energy transfer properties of anthryl-oligothienyl-porphyrins)

RN 3779-27-9 HCAPLUS
CN [2,2'-Bithiophene]-5-carboxaldehyde (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

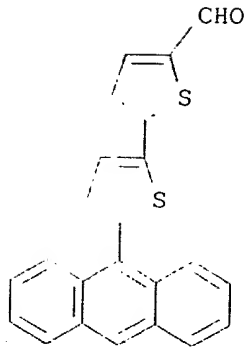


RN 7342-41-8 HCAPLUS
CN [2,2':5',2''-Terthiophene]-5-carboxaldehyde (7CI, 8CI, 9CI) (CA INDEX NAME)

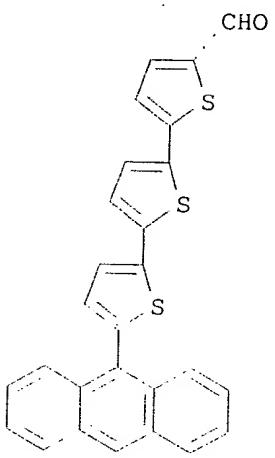


IT **165393-21-5P 165393-22-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and energy transfer properties of anthryl-oligothienyl-porphyrins)

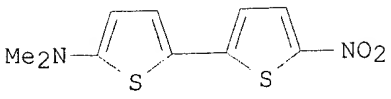
RN 165393-21-5 HCAPLUS
CN [2,2'-Bithiophene]-5-carboxaldehyde, 5'-(9-anthracenyl)- (9CI) (CA INDEX NAME)



RN 165393-22-6 HCAPLUS
CN [2,2':5',2''-Terthiophene]-5-carboxaldehyde, 5''-(9-anthracenyl)- (9CI) (CA INDEX NAME)



L71 ANSWER 13 OF 14 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1995:466000 HCAPLUS
DOCUMENT NUMBER: 123:32543
TITLE: Synthesis and Solvatochromic Properties of Donor-Acceptor-Substituted Oligothiophenes
AUTHOR(S): Effenberger, Franz; Wuerthner, Frank; Steybe, Felix
CORPORATE SOURCE: Institut fuer Organische Chemie, Universitaet Stuttgart, Stuttgart, D-70569, Germany
SOURCE: Journal of Organic Chemistry (1995), 60(7), 2082-91
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

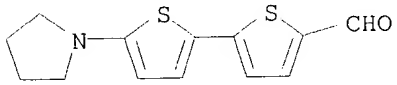


I

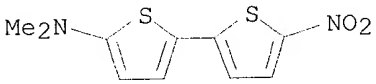
AB The Pd-catalyzed cross-coupling reaction of electron-donor-substituted thiophenes with electron-acceptor-substituted halothiophenes via organozinc intermediates or organotin compds. to give bi-, ter-, and quaterthiophenes is described. (Dimethylamino)bithiophenes with acceptor groups of varying reactivity were prepd. in 60-80% yield, whereas other bithiophenes were obtained as a mixt. with phenylthiophenes. Sym. substituted byproducts were formed in the conversion of 2-methoxythiophene with bromothiophenes via organozinc compds., yielding oligothiophenes. Ter- and quaterthiophenes were isolated in about 50-70% yield. The electronic interactions between donor and acceptor end groups in **conjugated** bithiophenes are expressed in the intense and markedly solvatochromic CT transitions. The solvatochromic behavior was detd. by linear regression analyses of absorption maxima in 11 solvents, whereby bithiophene I was found to be a very appropriate indicator dye, whose absorption wavenumbers in aliph. and dipolar aprotic solvents and, on consideration of the polarizability correction term d.delta., in arom. and chlorinated solvents excellently correlate with .pi.* values defined by Kamlet and Taft.

IT **146823-45-2P 149969-21-1P 150239-76-2P 150239-77-3P 163928-45-8P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and solvatochromism of donor-acceptor-substituted oligothiophenes)

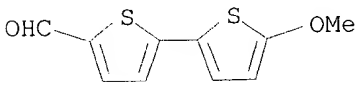
RN 146823-45-2 HCAPLUS
CN [2,2'-Bithiophene]-5-carboxaldehyde, 5'-(1-pyrrolidinyl)- (9CI) (CA INDEX NAME)



RN 149969-21-1 HCAPLUS
CN [2,2'-Bithiophen]-5-amine, N,N-dimethyl-5'-nitro- (9CI) (CA INDEX NAME)

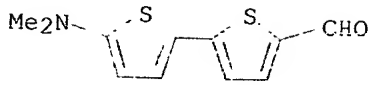


RN 150239-76-2 HCAPLUS
CN [2,2'-Bithiophene]-5-carboxaldehyde, 5'-methoxy- (9CI) (CA INDEX NAME)

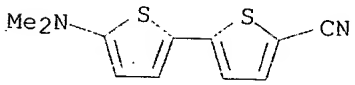


RN 150239-77-3 HCAPLUS
CN [2,2'-Bithiophene]-5-carboxaldehyde, 5'-(dimethylamino)- (9CI) (CA INDEX

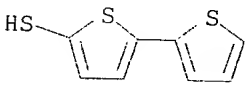
NAME)



RN 163928-45-8 HCAPLUS
CN [2,2'-Bithiophene]-5-carbonitrile, 5'-(dimethylamino)- (9CI) (CA INDEX NAME)



IT **159157-32-1**, 5-Mercapto-2,2'-bithiophene
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. and solvatochromism of donor-acceptor-substituted oligothiophenes)
RN 159157-32-1 HCAPLUS
CN [2,2'-Bithiophene]-5-thiol (9CI) (CA INDEX NAME)

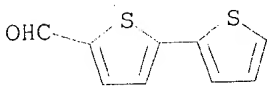


L71 ANSWER 14 OF 14 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1995:314954 HCAPLUS
DOCUMENT NUMBER: 122:132487
TITLE: Quadratic nonlinear optical properties of some donor-acceptor substituted thiophenes
AUTHOR(S): Hutchings, Michael G.; Ferguson, Ian; McGeein, David J.; Morley, John O.; Zyss, Joseph; Ledoux, Isabelle
CORPORATE SOURCE: Zeneca Spec. Res. Cent., Blackey, M9 8ZS, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1995), (1), 171-6
CODEN: JCPKBH; ISSN: 0300-9580
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A series of thiophenes and bithiophenes contg. combinations of dimethylamino and dimethyl-hydrazono .pi.-acceptor groups was synthesized in order to study their non-linear optical properties. Soln. mol. hyperpolarizabilities were detd. by a combination of exptl. dipole moments and results from the elec. field induced second harmonic generation expt. Values obtained correlate well with those calcd. by the CNDOVSB MO method. The main structure-property relationships deduced from the results are: (i) thiophene provides a more efficient electron delocalization pathway than benzene; (ii) this increase is proportionately even greater for bithiophene compared with biphenyl; (iii) dimethylhydrazono results in twice the hyperpolarizability of dimethylamino in a comparable mol.; and (i.v.) dicyanovinyl is a more effective electron acceptor group than nitro in the thiophenes synthesized and calcd.

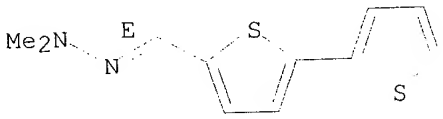
IT **3779-27-9P**, [2,2'-Bithiophene]-5-carboxaldehyde
160893-19-6P 160893-20-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(conversion to donor-acceptor substituted thiophenes with quadratic nonlinear optical properties)

RN 3779-27-9 HCAPLUS
CN [2,2'-Bithiophene]-5-carboxaldehyde (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



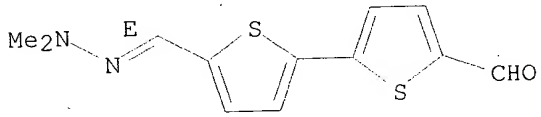
RN 160893-19-6 HCAPLUS
CN [2,2'-Bithiophene]-5-carboxaldehyde, dimethylhydrazone, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 160893-20-9 HCAPLUS
CN [2,2'-Bithiophene]-5,5'-dicarboxaldehyde, mono(dimethylhydrazone), (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



see the d que for L57 for explanation of this d que

TRAN 09/871,353

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=> d que l76
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L2         135 SEA FILE=HCAPLUS ABB=ON  PLU=ON  GIGLI G?/AU
L3         377 SEA FILE=HCAPLUS ABB=ON  PLU=ON  CINGOLANI R?/AU
L4          48 SEA FILE=HCAPLUS ABB=ON  PLU=ON  FAVARETTO L?/AU
L5          59 SEA FILE=HCAPLUS ABB=ON  PLU=ON  ZAMBIANCHI M?/AU
L6          78 SEA FILE=HCAPLUS ABB=ON  PLU=ON  SOTGIU G?/AU
L7          71 SEA FILE=HCAPLUS ABB=ON  PLU=ON  CITRO G?/AU
L8         132 SEA FILE=HCAPLUS ABB=ON  PLU=ON  BARBARELLA G?/AU
L9         734 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L1 OR L2 OR L3 OR L4 OR L5
               OR L6 OR L7 OR L8)
L10         54 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L9 AND THIOPHENE
L11         30 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L10 AND OLIGOMER?
L12          5 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L11 AND (THIOPHENE OLIGOMER)/T
               I
L13         24 SEA FILE=REGISTRY ABB=ON  PLU=ON  (376393-41-8/BI OR 376393-42-
               9/BI OR 376393-43-0/BI OR 376393-44-1/BI OR 492-97-7/BI OR
               111372-97-5/BI OR 111744-23-1/BI OR 113386-74-6/BI OR 116159-99
               -0/BI OR 118347-89-0/BI OR 127236-47-9/BI OR 127236-48-0/BI OR
               127473-73-8/BI OR 127473-74-9/BI OR 127473-75-0/BI OR 139747-07
               -2/BI OR 139747-08-3/BI OR 14762-74-4/BI OR 201604-95-7/BI OR
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               BI OR 67984-20-7/BI)
L14          4 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L12 AND L13
L15          5 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L12 OR L14
L16           STR
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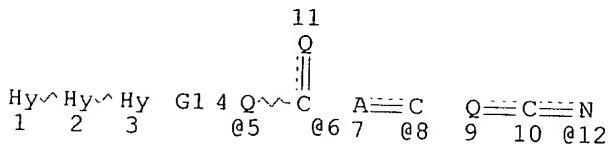


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VAR G1=5/6/8/12/NH2/OH/SH/SO3H/SO2
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
GGCAT   IS MCY  UNS  AT   1
GGCAT   IS MCY  UNS  AT   2
GGCAT   IS MCY  UNS  AT   3
DEFAULT ECLEVEL IS LIMITED
ECOUNT  IS E4 C  E1 S  AT   1
ECOUNT  IS E4 C  E1 S  AT   2
ECOUNT  IS E4 C  E1 S  AT   3

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  12

STEREO ATTRIBUTES: NONE
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L19           STR

Hy Hy Hy
1  2  3


NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
GGCAT   IS MCY  UNS  AT   1
GGCAT   IS MCY  UNS  AT   2
GGCAT   IS MCY  UNS  AT   3
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Searched by Susan Hanley 305-4053

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DEFAULT ECLEVEL IS LIMITED
ECOUNT  IS E4 C  E1 S  AT   1
ECOUNT  IS E4 C  E1 S  AT   2
ECOUNT  IS E4 C  E1 S  AT   3

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   3

STEREO ATTRIBUTES: NONE
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L23         2293 SEA FILE=REGISTRY SUB=L21 SSS FUL L16
L26              STR
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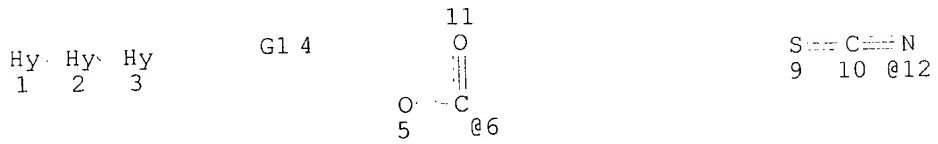

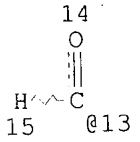


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VAR G1=OH/SH/NH2/13/6/12
NODE ATTRIBUTES:
CONNECT IS E1  RC AT   5
DEFAULT MLEVEL IS ATOM
GGCAT   IS MCY  UNS  AT   1
GGCAT   IS MCY  UNS  AT   2
GGCAT   IS MCY  UNS  AT   3
DEFAULT ECLEVEL IS LIMITED
ECOUNT  IS E4 C  E1 S  AT   1
ECOUNT  IS E4 C  E1 S  AT   2
ECOUNT  IS E4 C  E1 S  AT   3

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  13

STEREO ATTRIBUTES: NONE
L27        1357 SEA FILE=REGISTRY SUB=L23 SSS FUL L26
L28         476 SEA FILE=REGISTRY ABB=ON  PLU=ON  L27 AND  3 16.145.3/RID
L29         166 SEA FILE=REGISTRY ABB=ON  PLU=ON  L27 AND  4 16.145.3/RID
L30         104 SEA FILE=REGISTRY ABB=ON  PLU=ON  L27 AND  5 16.145.3/RID
L31         746 SEA FILE=REGISTRY ABB=ON  PLU=ON  (L28 OR L29 OR L30)
L32         674 SEA FILE=REGISTRY ABB=ON  PLU=ON  L31 AND NC=1 NOT ("DIAZO" OR
                F/ELS)
L72           6 SEA FILE=REGISTRY ABB=ON  PLU=ON  L32 AND  "ISOTHIOCYANATO"
L75           2 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L72
L76           1 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L75 NOT L15
```

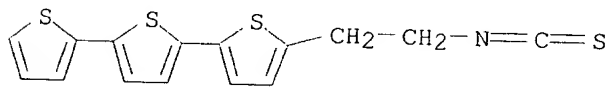
=> d ibib abs hitstr

L76 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:792698 HCAPLUS
DOCUMENT NUMBER: 136:66480
TITLE: Oligothiophene isothiocyanates as a new class of fluorescent markers for biopolymers
AUTHOR(S): Barbarella, Giovanna; Zambianchi, Massimo; Pudova, Olga; Paladini, Vanessa; Ventola, Alfredo; Cipriani, Francesco; Gigli, Giuseppe; Cingolani, Roberto; Citro, Gennaro
CORPORATE SOURCE: Consiglio Nazionale Ricerche, I.Co.C.E.A, Bologna, 40129, Italy
SOURCE: Journal of the American Chemical Society (2001), 123(47), 11600-11607
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

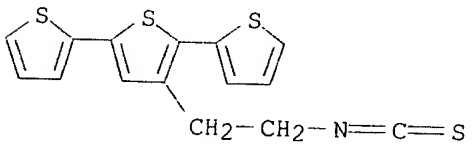
AB The regioselective synthesis of fluorescent oligothiophene isothiocyanates is described. The isothiocyanates were reacted with bovine serum albumin (BSA) following std. procedures and the optical properties of the oligothiophene-BSA conjugates were analyzed as a function of oligomer concn., time, and irradn. power. The oligothiophene-BSA conjugates were chem. very stable and their photoluminescence characteristics persisted unaltered for several months. Photoluminescence data relative to the conjugate of an oligothiophene-S,S-dioxide isothiocyanate with monoclonal anti-CD8 antibody are reported. No fluorescence quenching was obsd. following the binding of the isothiocyanate to the antibody and the conjugate displayed high chem. stability and photostability.

IT **376393-41-8DP**, reaction conjugated with bovine serum albumin
385369-25-5DP, reaction conjugated with bovine serum albumin
385369-31-3DP, reaction conjugated with bovine serum albumin
385369-34-6DP, reaction conjugated with CD8 antibody
RL: ARU (Analytical role, unclassified); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation)
(oligothiophene isothiocyanates as a new class of fluorescent markers for biopolymers)

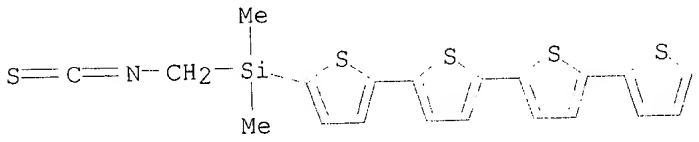
RN 376393-41-8 HCAPLUS
CN 2,2':5',2''-Terthiophene, 5-(2-isothiocyanatoethyl)- (9CI) (CA INDEX NAME)



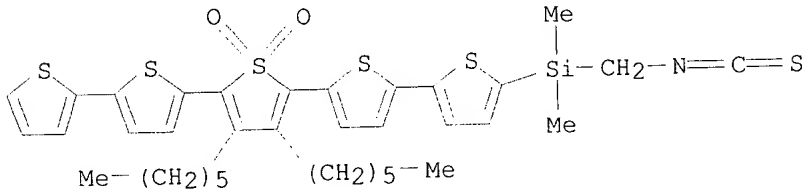
RN 385369-25-5 HCAPLUS
CN 2,2':5',2''-Terthiophene, 3'-(2-isothiocyanatoethyl)- (9CI) (CA INDEX NAME)



RN 385369-31-3 HCAPLUS
CN Silane, (isothiocyanatomethyl)dimethyl[2,2':5',2'':5'',2'''-quaterthiophen]-5-yl- (9CI) (CA INDEX NAME)



RN 385369-34-6 HCAPLUS
CN Silane, (3'',4'''-dihexyl-1'',1'''-dioxido[2,2',5':2'':5'',2''':5''',2''''-quinquethiophen]-5-yl)(isothiocyanatomethyl)dimethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT